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Non-linear 4-D Real Time Expert Seismology, Non-linear Singular Integral Operators Method & Artificial Lift for Oil-Gas Exploration & Well Development Suitable for the Major Petroleum Companies

by Evangelos Ladopoulos, President & CEO of EUAS

Short Biography

Prof. Dr. Civil Engineer, Mechanical (Aerospace) Engineer & Petroleum Engineer, D.Sc.
Included in the list of 2000 Outstanding Scientists of 20th Century by Cambridge Bio Centre.
Included in the list of 2000 Outstanding Scientists of 21st Century by Cambridge Bio Centre.
Included in the list of 100 Top Scientists of 2007 by Cambridge Bio Centre.
Over 300 publications in high quality scientific journals and 5 books.
Project Manager for over 500 Projects in Civil Engineering, Mechanical Engineering, Aerospace Engineering and Petroleum Engineering.
Chairman and Professor by Interpaper Research Organization.
Visiting Professor at Universities in Europe and USA.
Editor-in-Chief of many SCI Engineering Journals.
President & CEO of the EU Academy of Sciences.
Member by several Academies in USA.

The modern method *"Non-linear Real-Time Expert Seismology"* is investigated for the designation of the exact location of the on-shore and off-shore petroleum and gas reserves worldwide. So, the above "innovative" and "groundbreaking" technology is applied by using a non-linear 3-D elastic waves real-time expert system and hence, the oil and gas reserves can be successfully determined. Besides, exact 3-D images are produced of the underground topography of the area. The exact location of the oil and gas reserves may be designated in the special areas where anticlines occur. So, the above high innovative petroleum method is working under Real Time Logic for searching the on-shore and off-shore oil and gas reserves developed on the continental crust and on deeper water ranging from 300 to 3000 m, or even deeper. The proposed method can be used for the exploration of petroleum reserves in very deep depths, like 20,000 to 30,000 m. Also, 4-D seismic imaging is proposed, which incorporates many 3-D seismic surveys over the same reservoir at specified intervals of time. Furthermore, an "innovative" method is investigated in the area of 4-D multiphase flows for the determination of the properties of reservoir materials, when petroleum reserves together with water are moving through porous media. Then the estimation of the future oil production from the reservoir can be evaluated. Consequently, the above petroleum engineering problem is reduced to the solution of a non-linear singular integral equation, which is numerically solved by using the Non-linear Singular Integral Operators Method (N.S.I.O.M.). Besides a modern model is proposed for oil and gas well development, by using the "Non-linear ESP Artificial Lift Method". According to the proposed new sophisticated technology the ESP Artificial Lift

Method will be extended to non-linear form, by adding multiple pumps. So, the well will be able to handle very big flow rates which could be 500,000 bpd, or even up to 1,000,000 bpd.

A.1 Four-dimensional Non-linear Real-time Expert Seismology

The energy demand for petroleum and gas will increase up to 2030 by 50-60%, as it is increasing worldwide yearly at a pace of 1.5 to 2.0%. In addition, the total estimated petroleum all over the world in place stands today approximately at 1.5 trillion barrels, and with current petroleum consumption at 90 million barrels per day, the hydrocarbons in place are predicted to last for the next 40 years. Consequently, there is an absolute need by major petroleum companies to increase their stock by finding new oil and gas reserves. For this reason international petroleum companies should be looking into other alternatives, like to drill to ever deeper horizons and in the relatively unexplored ocean depths. It is known that oceans cover about 70% of the earth's surface and most of the waters are at more than 2000 m deep. Hence, major oil companies and scientific petroleum organizations are prepared for tapping into the relatively unknown areas with potential for large discoveries.

Energy is one of the largest economic domains globally. Our proposed innovative and groundbreaking method in the area of oil exploration, hence in the overall energy domain, will help improve our competitive role in the international scene. There are many seas around with a big amount of unexplored quantities of oil and gas in deep waters waiting to be explored. In such case the role of many countries worldwide should be emphasized and will be reduced their dependency from external sources.

As the recent theoretical and experimental evidence demonstrates the possibility that petroleum may have formed in the depths of the earth, then major oil companies must be ready to face the new challenges of drilling even deeper, to the basement rock, where very huge oil and gas fields may await to be discovered. Modern technologies will have therefore a major impact in the future. Through the technological progress to be achieved in the future exploration, then major reductions in costs can be very much expected. It is believed that the expected progress of enhanced oil recovery methods will reduce their future technical cost substantially. Consequently, it is absolutely sure that drilling depths will be increasing in the future and the industry should be geared up and ready for meeting the many challenges. According to the current research the drillings in the near future could reach the 20,000 m, or even the 30,000 m in the subsurface of earth.

On the other hand, since 1920 and for over a century the basic and prevalent theory on oil and gas reserves exploration, was *"Reflection Seismology"* and *"Refraction Seismology"*. According to the above methods the basic idea is to collect reflections of elastic (seismic) waves and then through various mathematical operations, by using Snell's law and Zoeppritz equations or the Kirchhoff equations to convert them to maps of the earth's structure. [1] - [9]. Hence, the methods of *"Reflection Seismology"* and *"Refraction Seismology"* for almost a century, have been used with several improvements for petroleum resources exploration.

By the current research for the on-shore and off-shore oil and gas reserves exploration the modern technology of *"Non-linear Real-Time Expert Seismology"* is investigated, as was recently proposed by E.G.Ladopoulos [12]-[15], [17]-[22], [24]-[31], [34]-[39], [42], [45]. So, *"Non-linear Real-Time Expert Seismology"* is a very "*innovative*" and "*groundbreaking*" method on petroleum and gas reserves exploration. According to the above modern technology a non-linear 3-D elastic waves real - time expert system is proposed for the exploration of petroleum and gas resources all over the world, including the off-shore petroleum reserves, of the seas and oceans in the whole world. The above new generic technology will work under Real Time Logic [46]-[50] for searching off-shore fuel reserves developed on the continental crust and on deeper water ranging from 300 to 3000 m, or even much more. Furthermore, the new exploration method will be the best device for searching the on-shore and off-shore hydrocarbon resources in very deep depths, even approaching 20,000 m or 30,000 m. By using therefore a new and very sophisticated model, then the exact location of the oil and gas reserves may be designated in the special areas where geological anticlines occur.

Consequently, the concept of the current research goes beyond other national and international RTD activities. For this reason, this research activity should be coordinated at a worldwide level and any improvements and applications of this technology should be

channelled through the big petroleum producers. The potential areas and markets of application of our research results will be the global oil market. The research results are applicable to all oil companies and scientific organizations working on oil exploration in the whole world. For maximum impact in the medium-/long-run, our proposed high technology should be applied by the oil companies for land and marine oil and gas exploration.

Additionally, through the new method exact 3-D images are produced of the underground topography of the area. Furthermore, 4-D imaging can be taken on a given area multiple times over an extended period of time. So, through the current research 4-D seismic imaging is proposed, which incorporates many 3-D seismic surveys over the same reservoir at specified intervals of time. Studying multiple time-lapsed 3-D surveys, or three-dimensional subsurface images, portrays the changes in the reservoir over time.

Consequently, there are many basic benefits for the new theory of "*Non-linear Real-Time Expert Seismology*" in comparison to the existing theories of *"Reflection Seismology"* and *"Refraction Seismology"*. These are the following:

a) The new method *"Non-linear Real-Time Expert Seismology"* is based on the special form of the geological anticlines, normal faults, reverse faults or deformations caused by intrusion of the bottom of the sea, in order to decide which areas of the bottom have the most possibilities to include hydrocarbon reserves. This is effected by using the proposed modern technology. On the other hand, the existing theory is only based to the best chance and do not include any theoretical and sophisticated model. Thus, currently international oil companies by using the existing methods of *"Reflection Seismology"* and *"Refraction Seismology"* must do a lot of expensive test drillings in big areas of seas, if they want to have a chance to find oil and gas reserves. As every deep drilling is too expensive, then every dry drilling would cost a lot of money to the oil companies.

b) The new proposed technology of elastic (sound) waves is based on the difference of the speed of the sound waves which are travelling through solid, liquid, or gas. In a solid the elastic waves are moving faster than in a liquid and the air, and in a liquid faster than in the air. On the other hand, existing theories are based on the applications of Snell's law and Zoeppritz equations or the Kirchhoff equations, which are not giving good results, as these which we are expecting by the new method.

c) The new method *"Non-linear Real-Time Expert Seismology"* is based on a Real-time Expert System working under Real Time Logic, that gives results in real time, which means every second. Existing theories do not include real time logic.

Reflection in Four-dimensional Non-linear Real-time Expert Seismology

Wavelength of the wave is the distance between two successive maxima (or between any two successive points in the same phase) and is denoted by l. Since the waveform, traveling with constant velocity u, advances a distance of one wavelength in a time interval of one period, then follows that the velocity of sound waves u is given by the following relation:

$$u = l\, v \qquad \text{(A.1.1)}$$

where v denotes the frequency.

So, it is clear, that the velocity u differs when the sound waves are traveling through solid, liquid, or gas. In a solid the elastic waves are moving faster than in a liquid and the air, and in a liquid faster than in the air. If searching for example for off-shore oil resources over the sea, by transmitting sound waves, then there will be a difference in the velocity of the waves in the sea, the solid bottom and in a potential reservoir.

In order the new technology to be better explained, consider the example of Figure 1. In the above example consider that in the bottom of the sea there is a potential oil reservoir. In this case, the speed of the elastic waves in the air (u_{air}), will be different from the speed in the water (u_{water}), and different from the speed in the solid bottom (u_{solid}) and different from the speed in the potential reservoir (u_{oil}), while the frequency of the elastic waves remaining the same when transmitted through every different matter.

Thus, by the current research a real - time non-linear 3-D plane - polarized elastic waves expert system is proposed in order to explore the on-shore and off-shore petroleum and gas resources, according to the new theory of *"Non-linear Real-Time Expert Seismology"*, in contrast to the old theory of *"Reflection Seismology"*.

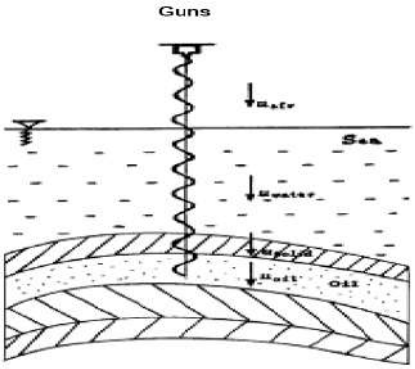

Fig. 1 Elastic Waves Method for the Exploration of Oil Reserves.

This modern and innovative Sound Waves Technology will work under Real Time Logic for searching off-shore petroleum reserves developed on the continental crust and on deeper waters ranging from 300 m to 3000 m, or even deeper and for very deep depths in the subsurface of earth up to 20,000 m or even to 30,000 m (Figure 2).

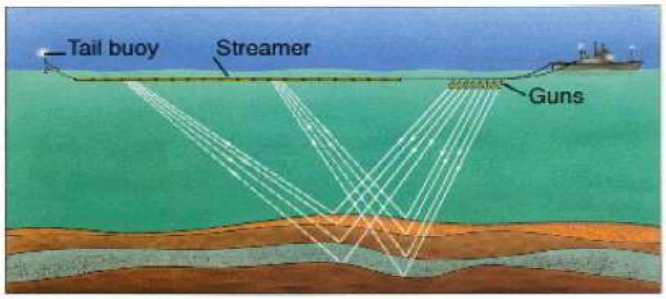

Fig. 2 Non-linear Real-time Expert Seismology.

The travel time T of the seismic waves is calculated as following:

$$T = \frac{2\left(d^2 + x^2/4\right)^{1/2}}{v} \tag{A.1.2}$$

in which d denotes the depth, x the distance between source of wave and the geophone or hydrophone detector and v is the average speed.

In addition, from (A.1.2) follows equation (A.1.3):

$$T^2 = \frac{4d^2 + x^2}{v^2} \tag{A.1.3}$$

Furthermore, the normal incident time T_o is given by the formula:

$$T_o = \frac{2d}{v} \tag{A.1.4}$$

From eqs (A.1.3) and (A.1.4) follows:

$$T^2 - T_o^2 = \frac{x^2}{v^2} \tag{A.1.5}$$

Consequently, from eqn (A.1.5) follows that the travel time curve for a constant velocity horizontal layer model is a hyperbola whose apex is at the zero-offset travel time T_o:

$$\frac{T^2}{T_o^2} - \frac{x^2}{(T_o v)^2} = 1 \tag{A.1.6}$$

Finally, from (A.1.5) the mean velocity is equal to:

$$v = \frac{x}{\sqrt{T^2 - T_o^2}} \tag{A.1.7}$$

A.2 Non-linear Singular Integral Operators Method for 4-D Petroleum Multiphase Flows

Petroleum well test analysis is a kind of a very important history matching process for the determination of the properties of reservoir solids. Thus, during the movement of petroleum reserves through porous media, then both single-phase and multiphase flow occurs. By the current research the multiphase flows are studied when the oil reserves are mixed with water. In addition, when a petroleum well test is conducted then the well is subjected to a change of its flow rate and the resulting pressure response is possible to be measured. Besides, this pressure is compared to analytical or numerical models in order to estimate reservoir parameters such as permeability. Then the estimation of the future oil production from the reservoir can be evaluated.

So, by using the Non-linear Singular Integral Operators Method (N.S.I.O.M.) [10], [11], [16], [23], [32], [33], [40], [41], [44] as proposed by E.G.Ladopoulos , then the pressure response in multiphase flows from the well test conducted in a heterogeneous reservoir will be computed. Besides, some properties of the porous medium equation, which is a Helmholtz differential equation, are proposed and investigated. Furthermore, basic properties of the fundamental solution will be analyzed and investigated.

In addition, 4-D multiphase flows can be taken on a given area multiple times over an extended period of time. Consequently, through the current research 4-D multiphase flows are proposed, which incorporates many 3-D flows over the same reservoir at specified intervals of time. Studying multiple time-lapsed 3-D surveys, or three-dimensional subsurface images, portrays the changes in the reservoir over time.

The benefits of the new method in comparison to existing methods are the following:

1. The new method is based on the N.S.I.O.M., by using non-linear singular equations. According to this theory the porous medium equation is reduced to the solution of a non-linear singular integral equation which is then numerically evaluated by using a non-linear programming method.

Existing methods of well test analysis, are using too as a start the porous medium equation, but as this is a complicated differential equation are giving only some analytical solutions for very simple cases or numerical solutions for homogeneous reservoir materials..

2. The new method, as it is a complicated non-linear numerical method can give results for heterogeneous porous media (which of course are the solids in reality) and not only for homogeneous solids as are giving the analytical or numerical existing methods.

So the estimation of the properties and the future petroleum production from a new oil reservoir could be done exactly, and not estimated as by the existing methods.

From the above two points it can be understood the evidence of the applicability of the new method, as it is based on non-linear software. Also its novelty, as it is based on the theory of non-linear singular integral equations. In general an oil reservoir well test in a single-phase reservoir is calculated by using the porous medium equation:

$$\nabla \bullet \left(\frac{\lambda}{\phi \xi} \nabla p\right) = c_t \frac{\partial p}{\partial t} \tag{A.2.1}$$

in which λ denotes the permeability, ϕ the porosity, ξ the viscosity, p the pressure of the reservoir, t the time and c_t the compressibility. By replacing variables as follows:

$$u = \left(\frac{\lambda}{\phi \xi}\right)^{1/2} p \tag{A.2.2}$$

then (A.2.1) can be written as:

$$\nabla^2 u + \lambda' u = 0 \tag{A.2.3}$$

Hence, (A.2.3) is a Helmholtz differential equation.

By applying the Green Element Method, then the problem reduces to the solution of a *non-linear singular integral equation*:

$$-\frac{\theta}{2\pi} p(r_i) + \int_{\partial\Omega} \left(p \frac{\partial[\ln(r - r_i)]}{\partial n} - \ln(r - r_i) \frac{\partial p}{\partial n} \right) dS +$$

(A.2.4)

$$+\iint_{\Omega}\ln(r-r_i)\left[-\nabla\ln\Lambda\bullet\nabla p+\frac{1}{\Lambda}\frac{\partial p}{\partial t}\right]d\Omega=0$$

In order the non-linear singular integral equation (A.2.4) to be numerically evaluated, then the Non-linear Singular Integral Operators Method (N.S.I.O.M.) will be used.

A.3 Non-linear ESP Artificial Lift Method by Multiple Pumps

Artificial lift is a process used on petroleum wells to increase pressure within the reservoir and encourage petroleum to the surface. When the natural drive energy of the reservoir is not strong enough to push the petroleum to the surface, artificial lift is employed to recover more production. While some wells contain enough pressure for oil to rise to the surface without stimulation, most don't, requiring artificial lift. In fact, 95% of the oil wells worldwide require artificial lift from the very beginning. Even those wells that initially posses natural flow to the surface, that pressure depletes over time, and artificial lift is then required. Consequently, artificial lift is generally performed on all wells at some time during their production life.

For the new and the existing oilfields there is an absolute need for the improvement of the existing methods of well development. For this reason, by the current investigation the *"Non-linear ESP Artificial Method by Multiple Pumps"* is proposed and investigated. According to the above new technology the ESP Artificial Lift Method will be extended to non-linear forms by adding multiple electric submersible pumps (ESP), in order to increase the production of each well to 500,000 bpd, or even up to 1 million bpd. The above multiple ESP pumps are used in a definite range of pumping rates. The new method has many benefits beyond the existing ESP Artificial Lift Method [51]-[53], as the oil production for each well is increased very much and so there no limits for the oil well production any more.

The power *P (*in *KW)* of an ESP pump is given by the following formula:

$$P=\frac{Q\left(\gamma H-p_{\text{int}ake}\right)}{\eta\cdot\eta_{surf}} \tag{A.3.1}$$

where Q is the pumping rate ($m^3/\sec$), H the head of the pump (m), γ is the specific gravity of the produced liquid (KN/m^3), $p_{\text{int}ake}(KN/m^2)$ is the pump suction pressure, called pump intake pressure, η is pump's efficiency and η_{surf} (usually 0.97) is the power efficiency of the surface equipment.

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Generalized Lorenz - Mie Theory Connections to Prof. Arthur Ashkin's Nobel Theory

by Gérard Gouesbet, Member EUAS

Short Biography

Professor Emeritus at the Rouen National Institute for Applied Science.

Research Topics.

I have been involved in several research topics, including the modelling of turbulent multiphase flows, nonlinear dynamics and chaos theory, both from experimental and theoretical points of view. My main commitment, however, concerns the topic of laser-light scattering theory and applications.

I particular, developed several generalized Lorenz-Mie theories (GLMTs) dealing with the scattering of illuminating arbitrary shaped beams with particles having a sufficient degree of symmetry to allow one to use a method of separation of variables. These theories allow one to bridge the gap between Rayleigh and ray optics regimes discussed by Arthur Ashkin when dealing with the interpretation of his experiments concerning optical levitation and trapping of macroscopic particles.

The most important ingredient in these GLMTs concerns the description of the illuminating beam and its encoding by coefficients known as Beam shape Coefficients (BSCs). These BSCs provide a way to use the Extended Boundary Condition Method (EBCM) to the scattering of arbitrary shaped beams by arbitrary shaped particles

Research Publications.

I have edited or authored several books, particularly "Generalized Lorenz-Mie theories" by Springer, co-authored with G. Gréhan, first published in 2011, with a second edition published in 2017.

I have authored or co-authored about 335 papers in Journals, and about 540 papers when including conference proceedings, as a whole about 990 communications (including conferences without any proceedings, patents, seminars, internal reports, contract reports).

***Records from Google Scholar Citations** (October 2018).*

Number of citations : about 12 200.

h-index: 56.

index i100: 27.

index i10: 231.

Conference Organizations.

I have participated to many committees of international conferences. My main commitment in this item, however, concerns the creation in 1987 of the Conference "Optical Particles Sizing", thereafter "Optical Particle Characterization" and eventually "Laser-light and interactions with particles". After Rouen, the conferences have been held in Phoenix, 1990 (USA), Yokohama, 1993 (Japan), Nürnberg, 1995 (Germany), Saint-Paul, 1998 (USA), Brighton, 2001 (England), Kyoto, 2004 (Japan), Graz, 2007 (Austria), Rouen, 2012 (France), Marseille, 2014 (France), Xi'An, 2016 (China), Texas A&M University, 2018 (USA). The next conference will take place in Warsaw, Poland (2020).

Awards.

Kyoto University 70th Anniversary Memorial Foundation Grant, 1988 (10 000 dollars).

« Chevalier des Palmes Académiques » (1990) : "Knight of a decoration for services of education".

Gold Medallion of Wroclaw university (Poland), received during the ceremonies of the 50th anniversary of the university (1995).

Best paper published in J. of radio-science (China),1995, for : K.F.Ren, G.Gouesbet, G.Grehan, Wang Yiping, generalized Lorenz-Mie theory and its application in particle sizing, Chinese journal of radioscience, 9, 2, 7-12, 1994 (in chinese).
Honorary professor of the north-eastern university,Shenyang, Liaoning, China, 1997. Ceremony on 30th may 1997.
Honorary professor of Xi-dian university, Xi-dian, China.
Price of the best paper of Xi-dian university for 1997 (relying on a citation index) for : K.F.Ren, G.Grehan, G.Gouesbet, symmetry relations in generalized Lorenz-Mie theory, Journal Optical Society of America A, 11, 6, 1812-1817, 1994.
Invited Commemorative Review Paper in a Special Issue of the journal Applied Optics, for its 50th Anniversary, as a member of the TOP50 list of most published authors.
Top downloaded paper over the last two years in Applied Optics in December 2013 : G.Gouesbet, J.A. Lock, List of problems for future research in generalized Lorenz-Mie theories and related topics, review and prospectus.
Most valued reviewers for the Journal of Quantitative Spectroscopy and Radiative Transfer. 2016.
Outstanding reviewer for Optics Communications. 2016.
Honorary member of ASFERA (Association Française d'Etudes et de Recherches sur les Aérosols). 2017.
Outstanding and recognized reviewer for the Journal of Quantitative Spectroscopy and Radiative Transfer. 2016. 2017.
Honorary associate editor of Journal of Quantitative Spectroscopy and Radiative Transfer. 2018.

Van de Hulst Recommendation.

In his introduction (Hints from History : A Foreword) to the book "Light scattering by nonspherical particles", edited by M.I.Michenko, J.W. Hovenier and L.D. Travis, Van de Hulst wrote (p XXIX) : "In more recent work on Mie theory two developments please me most : (a) the many papers, mainly by Gouesbet and co-workers, on scattering of a focused (laser) beam that illuminates the sphere eccentrically (b) the glare points…".

My research started with the building and use of a laser Doppler velocimeter (LDV) to measure the velocity of laminar and turbulent liquid flows (1973). I thereafter used an improved LDV system to measure the velocity of a thermal plasma, in which the atom temperature was 5000 K and the electron temperature was 10 000 K (1977), with particles injected in the plasma. During this study, I had to deal with a frustration, namely that it would have been more secure to simultaneously measure simultaneously the velocity and size of individual particles transported by the plasma, something which was impossible at this time. This led me to the issue of optical particle characterization and, in order to design instruments and interpret data, to the building of a theory known as GLMT, i.e. generalized Lorenz-Mie theory [1].

GLMT *stricto sensu* describes the interaction between a laser beam and a homogeneous spherical particle. More generally, GLMTs describe the interaction between a laser beam and particles having a sufficient amount of symmetry to solve the problem by using the method of separation of variables. These theories allow one to compute scattered amplitudes and intensities, internal amplitudes and intensities, and optical forces and torques. They have been applied to many fields including optical particle characterization techniques (such as phase Doppler instruments, imaging, rainbow refractometry, to name a few), study of morphology-dependent resonances, mechanical effects of light, nonlinear effects, quantum mechanics in microcavities, scattering phenomena for particles illuminated by ultra-short femtosecond pulses. The reader may refer to a textbook [2] and to a recent review paper [3].

In GLMTs, the laser is described by using expansions of the electric and magnetic fields over vector wave functions, with expansion coefficients expressed in terms of beam shape

coefficients (BSCs). When dealing with the interaction between laser beams and complex particles which cannot be analyzed by using the method of separation of variables, such as by using the extinction boundary condition method (EBCM), these BSCs which are ingredients of GLMTs have to be used as well. This extends the applications of GLMTs and GLMT ingredients to a larger scope, e.g. [4].

In October 2018, Arthur Ashkin received a Nobel prize for his many works, in particular those dealing with optical levitation, optical trapping, optical tweezers and optical manipulation of macroscopic particles. From a theoretical point of view, Ashkin's experiments have been discussed by distinguishing two kinds of optical forces, namely scattering forces which are proportional to the optical intensity and points in the direction of the incident light, and gradient forces which are proportional to the gradient of the intensity and points in the direction of the intensity gradient. This decomposition of optical forces is carried out both in the Rayleigh regime (small particle size with respect to the wavelength) or in the ray optics regime (large particle size with respect to the wavelength).

The line of research of Arthur Ashkin meets the GLMT line at two intersections. First, because GLMTs are rigorous theories based on Maxwell's equations, they bridge the gap between the Rayleigh and ray optics regimes, allowing one to rigorously and analytically deal with optical forces and torques, with a host of applications in optical trapping of various kinds of particles. Second, optical levitation experiments have been carried out to test the predictions of the GLMT *stricto sensu*. A general review devoted to GLMTs and mechanical effects of light, as a celebration of Arthur Ashkin's pioneering work in optical levitation and manipulation is on the way [5].

I had a few other research fields from which I would select (i) modeling of turbulent two-phase flows (ii) instability of free surface locally heated and (iii) nonlinear dynamics and chaos theory.

Concerning the modeling of turbulent two-phase flows, it dealt with the theoretical study and computer simulation of the behaviour of discrete particles embedded in turbulent flows. A first step concerns the simulation of the turbulent flow itself. In a second step, the behaviour of particles in the simulated flow can be studied by using either an Eulerian or a Lagrangian approach. In the Eulerian approach, particles are pretended to constitute a scalar field whose behaviour is driven by a dispersion process governed by a dispersion tensor. In the Lagrangian approach, trajectories of individual particles are built in the flow by using a Newton law and the formulation of different forces acting on the particles. The most significant applications of such studies likely concern turbulent spray combustion. My last synthesis on this issue is Ref.[6].

Another line of research (ii) concerns the discovery of the oscillations of a thermal lensing when a laser beam propagates, under certain circumstances, below the surface of a liquid. These oscillations, called optical heartbeats, produce a host of behaviours known as period-doubling bifurcations, quasiperiodic oscillations and even chaos in the language of nonlinear dynamics theory. Experiments under zero gravity conditions helped to the understanding of these phenomena. A variant used a hot-wire located below the surface, leading to the observation of a new class of propagating waves, and to a new class of spatio-temporal 1D-phenomena, or to the observation of type-II intermittency in a hydrodynamic system. Experiments have been the opportunity to theoretically study instabilities produced both by buoyancy and surface tension effects in a horizontal liquid layer, leading to overstability and exchange of stability phenomena. These studies have been summarized, together with open questions, in Ref.[7].

As a result of such experimental studies related to instabilities and nonlinear dynamics, I have also been involved in bifurcation, nonlinear dynamics, and chaos theory (iii). My

main achievement in this field has been the building of an algoritm allowing one, from experimental scalar time series, to reconstruct the equations of motion of the system studied in a reconstructed phase space, a field known as global reconstruction of dynamical systems. My research in this field has been summarized in a book containing a comprehensive review paper from my group, together with a few papers from other groups [8].

I also dealt with a few miscellaneous issues, including kinetic theory of gases under high temperature conditions, experiments in combustion, dynamics light scattering (diffusion broadening spectroscopy, photon correlation spectrocopy, quasi-elastic light scattering spectrocopy) and properties of soot particles, microholography, particle size measurements using a top-hat beam technique or a double visible/infrared laser system, radiative transfer using either four-flux models or Monte-Carlo simulations for multiple scattering media, failure of the optical theorem both for electromagnetic (vectorial) and quantum (scalar) waves, and generalization of the optical theorem under circumstances (structured beams) where it lacks of generality, necessity of dealing with the theory of distributions in the framework of some light scattering problems, knot theory for the study of unstable periodic orbits in strange attractors, Hamiltonian chaos…

Finally, I fairly recently developed a strong interest to philosophy and history of science, particularly to the Duhem-Quine underdetermination of theories by experiments [9] and to the famous Bohr/Einstein debate (or say Copenhagen interpretations/hidden variables interpretations) in quantum mechanics [10].

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Advanced Materials for Energy Storage & Conversion

by Zongping Shao, Member EUAS

Short Biography

Zongping Shao is a professor of chemical engineering at Nanjing Tech University, China and Curtin University, Australia. He obtained his PhD from Dalian Institute of Chemical Physics, China in 2000. He worked as a visiting scholar at Institut de Researches Sur La Catalyse, CNRS, France from 2000 to 2002, and a postdoc at California Institute of Technology, USA from 2002 to 2005.

Research Activities and Publications

Professor Shao's research interests include oxygen permeable membranes, solid oxide fuel cells (SOFCs), oxygen reduction, oxygen evolution and hydrogen evolution reactions (ORR, OER and HER), lithium-ion batteries, supercapacitors, polymer-electrolyte membrane fuel cells, solar cells, etc. He has published more than 500 international journal papers with a total citation of >22000 and an H-index of 69 (Google Scholar). He was selected by Thomson Reuters as one of the highly cited researchers in the engineering section (2014 and 2017). He was also awarded as one of the highly cited Chinese researchers in the energy section by Elsevier China (2015-2017).

Selected Awards and Honors

1. *Second Prize in Hubei Province Science and Technology Award, China, 2017*
2. *Highly Cited Researcher, Thomson Reuters, 2017*
3. *The Member of EU Academy of Sciences, 2017*
4. *Millions of Talent Projects National Candidates, China, 2017*
5. *Special Government Allowances of the State Council, China, 2016*
6. *Second Prize in Jiangsu Province Science and Technology Award, China, 2015*
7. *Highly Cited Researcher, Thomson Reuters, 2014.*
8. *Distinguished Award for Novel Materials and their Synthesis by IUPAC& NMS, 2013*
9. *ARC Future Fellowships, 2011*
10. *The Changjiang (Yangtze River) Scholar Award, Chinese Ministry of Education, 2011*
11. *National Science Foundation for Distinguished Young Scholars of China, 2010*
12. *Young Researcher New Star Scientist Award (Scopus), 2010*
13. *"New Century Scientist" Awarded by Chinese Ministry of Education, 2008*
14. *Outstanding Young Scholar Award from Jiangsu Province, China, 2008*
15. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2008*
16. *Fok Ying Tung Research Grant for Excellent Scientist under 35, Education Foundation, Hong Kong, 2007*
17. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2007*

18. *First Prize of Advance in Science and Technology of Liaoning Province, China, 2006*
19. *K.C. Wang Scholarship for Young Chinese Researchers Abroad, 2001-2002*
20. *President Prize of Chinese Academy of Sciences, 2000*
21. *Excellent Undergraduate Student of Hangzhou University, China, 1995*

Major Research Areas

1. Mixed conducting membranes for the oxygen permeation
2. Key materials for SOFCs
3. Electrocatalysts for the ORR, OER and HER
4. Lithium-ion batteries and supercapacitors

Typical Researches

$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), a mixed oxygen-ionic and electronic conductor, was initially developed by Z. P. Shao as a ceramic membrane for oxygen separation from air. In 2004, Z. P. Shao applied BSCF, for the first time, as a cathode material for SOFCs operated below 600 °C. Since then, extensive research has been conducted on intermediate temperature (IT)-SOFCs all over the world. Actually, BSCF has become the hottest cathode material of IT-SOFCs nowadays. This is clearly indicated by the high citations of the paper (***Nature***, 2004, *431*, 170-173; 1965 times until October, 2018). Afterwards, Prof. Shao's group continues to develop novel cathode materials for IT-SOFCs, for example, $SrSc_{0.2}Co_{0.8}O_{3-\delta}$, $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$, and $PrBaCo_2O_{5+\delta}$. The operation temperature of SOFCs was further reduced to the range of 400-600 °C, promoting the development of low-to-intermediate temperature SOFCs.

Prof. Shao has also developed perovskite-based anode materials for SOFCs that can address the coking/sulfur poisoning of the conventional nickel cermet-based anode. The use of a water-storable proton-conducting perovskite oxide as the ceramic phase in the nickel-based anode was found to rapidly eliminate as-deposited carbon/sulfur, leading to the spontaneous regeneration of the nickel surface and the prevention of the carbon/sulfur accumulation. Furthermore, the potential of combining nanocatalysts and water-storable materials in advanced anode catalysts for SOFCs was demonstrated by using a facile impregnation and limited reaction protocol. A hierarchical anode composed of nickel nanoparticles, water-storable $BaZr_{0.4}Ce_{0.4}Y_{0.2}O_{3-\delta}$ perovskite, and amorphous BaO exhibited high hydrogen electro-oxidation activity, excellent operational stability, and superior sulfur tolerance.

For the room-temperature ORR, Prof. Shao introduced an effective strategy to boost the electrocatalytic activity of palladium (Pd) by stabilizing its unusual oxidation states. $LaFe_{1-}$

$_xPd_xO_3$ (x = 0.05 and 0.1) perovskite oxides (containing perovskite-type ionic, $Pd^{3+/4+}$) were prepared by doping Pd into the perovskite oxide lattice, showing higher mass activity, better durability, and stronger tolerance to methanol than the benchmark Pt/C (platinum supported on carbon). In addition, the introduction of A-site cation deficiency was demonstrated as another approach to enhancing the ORR activity of $LaFeO_3$, which is associated with the creation of oxygen vacancies and Fe^{4+} species.

For the OER electrocatalysis, Prof. Shao utilized a doping or co-doping strategy to develop several highly active and stable perovskite electrocatalysts, such as $SrNb_{0.1}Co_{0.7}Fe_{0.2}O_{3-\delta}$, $BaCo_{0.9-x}Fe_xSn_{0.1}O_{3-\delta}$, and $SrCo_{0.95}P_{0.05}O_{3-\delta}$. These catalysts feature well-tailored catalytically active sites and show OER activities that are comparable to or even better than the state-of-the-art precious metal-based IrO_2. A magnetron sputtering method was further adopted by Prof. Shao to construct amorphous perovskite nanofilms loaded on nickel foam substrate, which gave rise to two orders of magnitude enhancement in OER mass activity. Such amorphous nanofilms can undergo fast reconstruction during electrocatalysis, which was proved to be a universal strategy toward the design of efficient OER catalysts. Very recently, Prof. Shao found that antiperovskite materials (e.g., $CuNNi_3$) represent another type of active catalysts for the OER.

For the HER electrocatalysis, Prof. Shao was the first to demonstrate the capability of perovskite oxides in catalyzing the HER in an alkaline solution. Through a facile A-site praseodymium (Pr) doping into the parent BSCF, he developed $Pr_{0.5}(Ba_{0.5}Sr_{0.5})_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ with well-tuned surface electronic structures and properties, performing competitively with other non-Pt catalysts. Furthermore, novel synthetic methods (e.g., electrospinning, exsolution) were used to develop several nanostructured perovskite-based HER catalysts, which leads to even better catalytic performance.

For supercapacitors, Prof. Shao designed perovskite-type $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$ (SCN) and reduced $PrBaMn_2O_{6-\delta}$ (r-PBM) as novel anion-intercalated electrode materials in an aqueous KOH electrolyte, showing high capacitance, excellent rate capability, and favorable cycling stability. This suggests that SCN and r-PBM perovskites have the potential to be promising electrode materials for next-generation supercapacitors.

Career-Best Research Outputs

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Nanostructured Ceramics, Ceramic Foams and Interpenetrating Composites

by Jon Binner, Member EUAS

Short Biography

Current Positions

Jan 2014 –	*Deputy Head, College of Engineering and Physical Sciences, University of Birmingham.*
Jan 2014 –	*Professor of Ceramic Science and Engineering, School of Metallurgy and Materials, University of Birmingham*

Previous Positions

Aug 2011 – Dec 2013	*Dean, School of Aeronautical, Automotive, Chemical & Materials Engineering, Loughborough University, UK*
Aug 2005 – July 2011	*Head of Department, Department of Materials, Loughborough University, UK*
Mar 2000 – Dec 2013	*Professor of Ceramic Materials, Department of Materials, Loughborough University, UK*
Apr 1999 – Mar 2000	*Professor of Materials Engineering and Head of Dept, Department of Materials Engineering, Brunel University, UK.*
Aug 1998 – Mar 2006	*Director, CERAM – University Collaboration, CERAM Research, Stoke on Trent, UK*
Aug 1998 – Mar 1999	*Reader, Dept. of Materials Engineering & Materials Design, University of Nottingham, UK.*
Aug 1994 – Jul 1998	*Senior Lecturer, as above*
Jan 1989 – Jul 1994	*Lecturer, as above.*
Aug 1985 – Dec 1988	*Temporary Lecturer, Dept. of Ceramics, University of Leeds, UK.*
Aug 1984 – Jul 1985	*Visiting Assistant Professor, Department of Materials Science and Engineering, University of California at Los Angeles, USA.*

Key Positions

I am currently the Deputy Head of the College of Engineering and Physical Sciences and the Professor of Ceramic Science and Engineering at the University of Birmingham (UoB). Prior to this, I have been a Dean and, twice, a Head of Department. I was the President of the Institute of Materials, Minerals & Mining, UK, from Jan 2013 – Dec 2014 and Past-President from Jan 2015 – Dec 2016. I am the current President-Elect for the European Ceramic Society and an Invited Member of the EU Academy of Sciences.

Research

The focus of my research is the generation of both the necessary scientific understanding and the required engineering solutions for the development of processing routes for advanced ceramic materials and composites that display technical and/or financial advantages over existing processes and which yield new or improved materials.

Research Income and Staff

- *129 research grants totalling ~£16.5M.*
- *35 PhD students and 2 MPhil students have been supervised to successful completion; 6 more PhD students are currently being supervised.*
- *38 Postdoctoral Research Fellow projects have been supervised with 5 currently ongoing.*

Publications Highlights

- *~218 research papers and 7 patents published.*
- *Editor of 9 books/conference proceedings and contributor to 10 more.*
- *Editor of Advanced Ceramics Report, Jan 1985 – Dec 1998.*
- *Member of the Editorial Board, Advances in Applied Ceramics, 2000 – present.*
- *Member of the Editorial Board, Journal of Materials: Design & Applications, IMechE, 1999-2003.*
- *One of a team of authors of the UK's Advanced Ceramics Foresight document.*

Recognition *(partial list)*

- *Institute of Materials Holliday Prize, 1995.*
- *Institute of Materials, Minerals and Mining Ivor Jenkins Medal, 2007.*
- *Institute of Materials, Minerals and Mining Verulam Medal and Prize, 2011.*
- *MBDA Innovation Award, 2016.*
- *Member of the EPSRC Peer Review College in the UK since 2000 and of the Engineering Strategic Advisory Team since 2015 (Chair from 2018).*
- *Association of Microwave Power in Europe for Research and Education, AMPERE, Fellow (one of only five worldwide over the 24 years AMPERE has existed)*
- *Honorary Professor, Kunming University of Science & Technology, China since Sept 1999; Honorary Professor, Beijing University of Chemical Technology, China, since Nov 2006.*
- *Around 65 keynote, plenary and invited talks have been given at conferences; twice my paper has received a prize for being the best paper at a conference and in 2013 one of my papers was judged to be the best over two-year period 2012-13 by the Journal of the European Ceramic Society; the leading ceramics journal worldwide based on impact factor.*
- *Research proposal referee for the EPSRC, UK; Australian Research Council; Deutsche Forschungsgemeinschaft; Estonian Research Council; National Science Foundation, USA; Science Foundation, Arizona, USA; Singaporean Science & Engineering Research Council; South African Foundation for Research Development; the US-Israeli Science & Technology Foundation*
- *Member of the Robert L. Coble Award for Young Scholars Award Committee, ACerS, 2016 – present*

The focus of the research is the generation of both the necessary scientific understanding and the required engineering solutions for the design and development of ceramic-based materials and process routes that display technical and/or economic advantages over existing approaches. The range of products worked on ranges from nanostructured to traditional ceramics, interpenetrating composites to ultra-high temperature ceramic matrix composites. This work, which has been ongoing since 1981 has led to the publication of 218 reviewed papers as well as 7 patents. It has involved 35 PhD students, 2 MPhil students and 38 postdoctoral researchers. The current team consists of a further 6 PhD students and 5 postdoctoral researchers. Work on three of the themes investigated is outlined below.

Nanostructured ceramics: This work was undertaken largely over the period 2000 – 2013, reducing very significantly in the level of activity when I moved from Loughborough University to the University of Birmingham (1st Jan 2014) since I had to leave most of my facilities behind. The work focused on producing and characterising a range of nanostructured ceramics, including alumina and zirconia toughened alumina, barium titanate, hafnium diboride and carbide, yttrium aluminium garnet (YAG) and a range of yttria partially stabilised zirconias, with the zirconia being the most developed. As a result of the work, it became possible to produce fully dense, genuinely nanostructured yttria tetragonal zirconia polycrystal (YTZP) ceramic from powders as fine as 20 nm; this is smaller than the size of a typical virus. Figure 1 shows conventional and nanostructured YTZP at the same magnification. The grain size of the nanostructured material is approximately 65 nm. The YTZP ceramics were found to display some extremely useful properties. For example, although zirconia is one of the strongest and toughest advanced ceramic materials, it is very vulnerable to attack by moisture, particularly at temperatures in the range ~100 – 300°C. The moisture causes a catastrophic phase change that can reduce conventional, submicron zirconia into a pile of damp powder in less than one hour at ~250°C. Whilst more resistant grades are being developed elsewhere, the new nanoYTZP has been found to show no trace whatsoever of the phase change even beginning to occur after 3 weeks at 250°C. Combined with high strength and, for the right grades, high toughness or ionic conductivity, this has led to significant interest being shown in these materials for applications as diverse as hip replacement implants, dental ceramics, solid oxide

fuel cell electrolyte and valves for the petrochemical industry.

The work was able to progress thanks to a series of research grants from EPSRC and the (then-named) TSB in particular, in combination with excellent industrial support. The Powders Sector of the Materials KTN (formerly PowdermatriX) also aided this process very much. Two EPSRC programmes and a DTI (now BEIS) project over the period 2002 – 07 got the work off to an excellent start and allowed the basic green forming and densification routes to be developed. The work then continued with an EPSRC Follow-on Fund project, which assessed the potential for commercial exploitation of the technology, before being developed further and broadened in terms of the range of ceramics being investigated via a TSB Collaborative Research project. The team were then able to capitalise on the developments and start to translate them into industry via support from the EPSRC Collaboration Fund. This grant allowed a nanozirconia engineering component prototype, the ceramic internals for a petrochemical valve, to be produced. Further support focused on scale up was received from the Royal Society Brian Mercer scheme, whilst additional TSB support was received for work in the area of bioceramics. This sequence of research grants, and the wonderful technology transfer nature of the EPSRC Follow On Fund and Collaboration Fund, really helped the team to accelerate the process of getting their ideas into industry.

Ceramic foams and interpenetrating composites: Largely working during the 1990s, low density ceramic foams made from a wide range of ceramic materials, both oxide and nonoxide, were made by a new process route based on gel casting. Applications ranged from thermal insulation, kiln furniture, hot gas filters and catalyst supports to interpenetrating composites and biomedical uses such as maxillofacial reconstruction amongst others.

The patented process for fabricating the ceramic foams, which was taken to full commercial status by Dytech Corporation Ltd based near Sheffield in the UK, involved the creation of a stable, well-dispersed, high solids content, aqueous ceramic suspension that also incorporated an acrylate monomer together with an initiator and catalyst. The latter is used to provide *in-situ* polymerisation. After the further addition of a foaming agent, a high shear mixer is used to provide simple mechanical agitation that results in the formation of a wet ceramic foam that can be dried and then fired. One of the advantages of this *in-situ* polymerisation method is that it is common to observe a period of inactivity between the addition of reagents and the actual beginning of the polymerisation reaction. This is known as the induction period or idle time (t_i) and is beneficial since it allows the casting of the fluid foam into a mould prior to polymerisation and control over the pore size. A wide range of ceramic materials were produced as foams using the new process. Although the majority of work has focused on the engineering ceramic oxides, materials such as alumina, cordierite, mullite and zirconia, a large number of other ceramics were able to be foamed. These include the bioceramic hydroxyapatite, the electroceramic lead zirconate titanate (PZT), low thermal expansion sodium zirconium phosphate (NZP) and non-oxides such as silicon carbide and aluminium nitride. In general, foams in the range 5% to 40% of theoretical density can be produced; a typical micrograph showing the structure can be seen in figure 2. Note how the pore walls and struts are solid and fully dense; this provides high strength and chemical resistance. Although the lower the density of the foam the larger the cell or pore size, research eventually allowed a far greater degree of control to be achieved. Foams could finally be produced with cells as large as 1 mm and densities as high as 20% of theoretical, whilst 30% dense foams were produced with cells as small as 20-50 μm. Foams made of the engineering ceramics such as alumina offer comparatively high strengths, up to 80 MPa crush strength and 25 MPa modulus of rupture. Thermal insulation is almost as good as fibre-based products whilst also offering a totally fibre- and dust-free working environment. With zirconia the service temperature can be as high as 2000^{o}C. A wide range of component shapes is also available. The production route itself is intrinsically a casting process and hence tiles, tubes and a range of other custom shapes can all be produced very easily. In addition, both the green and fired foam may be readily machined, drilled, turned and slit opening up the possibility of producing some very complex shapes indeed. Figure 3 illustrates just a small selection of the shapes that have been produced. In addition, it is a simple process to apply a dense coating to one or more surfaces, either to eliminate permeability or to increase the mechanical properties of the surface layers. One application that could utilise this is

the production of ultra-low mass ceramic crucibles. These can significantly reduce the thermal mass to be heated during processing of their contents, thus improving energy efficiency.

This work subsequently led to the creation, during the first decade of this century, of interpenetrating composites, which are a new kind of composite structure in which there is an interpenetrating matrix of two different phases, in this case ceramic with either metal or polymer. They are also known as 3-3 composites, where the numbers refer to the number of dimensions in which each phase is continuous. It is the open porous structure of the foams that allows them to be infiltrated relatively easily with either molten metals such as aluminium or magnesium or any number of polymeric materials, though much more work was undertaken into creating metal-ceramic interpenetrating composites (IPCs) than their polymeric equivalents. Initially made by squeeze casting the metal into the ceramic foam, the ability to control the wetting angle was developed and this allowed pressureless infiltration to be achieved. This significantly increased the ability to make more complex structures. The ability to combine useful properties from metals, polymers and ceramics led to a wide range of potential applications for the composites, from electrically conductive wear resistant materials, through to interfacial materials for use in armour and, for the polymer-ceramic composites, sonar. For example, most armour systems are made up of composite layers of a number of materials to obtain the maximum protection for the minimum mass. However, when there is a ceramic front face, acoustic impedance mismatches at the resulting interface can be a cause of significant problems since the stress waves from the ballistic event are reflected back inside the ceramic as tensile waves, causing its rapid destruction. Ceramic-faced, metal–ceramic IPCs were produced *in-situ* using a pressureless infiltration technique so that a thin layer of metal bonded the front face to the IPC. Extensive work on characterising the impact performance of the components was undertaken using both a laboratory-based high strain rate approach (split Hopkinson pressure bar, SHPB) and actual ballistic tests using steel tipped, 7.62 mm, armour piercing rounds. The results of the latter showed that, whilst the expected damage was sustained by the front face, there was zero depth of penetration – even though the front face was only 4 mm of laboratory-standard alumina, rather than ~10 mm of armour-grade alumina. It is believed that the IPC layer provided a reduction in the impedance mismatch between the ceramic front and the aluminium alloy backing. The plastic deformation in the IPCs was observed to result from the presence of dislocations allowing the metal phase to deform whilst the ceramic phase coped with the distortion via localised cracking. The presence of metal bridges across the crack fronts helped to increase the damage tolerance in the IPCs.

Ultra-high temperature composites: Work undertaken since about 2010 has focused more on the creation of composites that can survive extreme conditions. Interest in advanced materials with a temperature capability over 2500°C for a range of aerospace applications involving launch and/or re-entry into Earth's atmosphere has increased over the last few decades. The most promising lightweight materials are carbon/carbon (C/C) composites due to their excellent high-temperature strength in reducing or neutral atmospheres, high thermal conductivity, low coefficient of thermal expansion (CTE) and excellent thermal shock resistance; however, they suffer badly from oxidation in air, even at temperatures below 1000^{o}C. There is thus a critical need to improve their oxidation and ablation resistance. Via funding from UK organisations such as the Defence Science & Technology Laboratories (DSTL), the Engineering & Physical Sciences Research Council (EPSRC), commercial organisations such as the European defence manufacturer MBDA and, more recently the EC's H2020 programme, has resulted in the development of C/C composites containing ultra-high temperature ceramic powders such as zirconium and hafnium diboride since these have been shown to be capable of protecting the composites even to temperatures as high as nearly 3000^{o}C. The mechanism by which they do this is still the subject of investigation by the team but a theory has been developed that requires the viscosity of the molten oxide to be measured; this is being undertaken in collaboration with CNRS in Orleans, France. Work has

focused on optimising the composition of the composites, their structure and optimising the amount of UHTC in the carbon fibre preforms; too little and the preform is not sufficiently protected, too much and the component's mass is unnecessarily high. As well as being able to make composites that can survive testing under conditions of almost 3000^{o}C, with heat fluxes up to 17 MWm^{-2} and gas velocities up to Mach 0.65, figure 4. As well as developing the materials, in recent years the work has focused on producing components with the production of both large panels and a complex-shaped jet vane, figure 5. The latter was tested both mechanically and thermos-ablatively and passed both tests.

The most recent programme, the European Commission-funded C3HARME project, has focused on extending the capabilities of the composite further, particularly in terms of manufacturing efficiency, reliability, cost-effectiveness and scalability. The project is based on the design and development of materials for applications as low-erosion nozzle inserts and thermal protection tiles for rocket launch and re-entry operations with the goal of achieving Technology Readiness Level, TRL, 5. The process is based on the use of chemical vapour infiltration, CVI. Conventionally, this process yields high quality parts but is a very slow process – it can take 2 – 3 months to make components. The latter can make them too expensive for their end-application. Work in the team is focused on accelerating this process using either RF heating (for carbon fibre-based composites) or microwave heating (for silicon carbide fibre-based composites – the latter are being examined for potential applications in aeroengines via funding from the US Air Force). Both types of heating can yield an 'inverse temperature profile', i.e. the centre of the composite is hotter than the surface. This means that the process can be speeded up and the latest results suggest that 3 – 4 days for manufacture is going to be quite possible; significantly faster than 2 – 3 months. This should bring down the manufacturing costs significantly, hopefully opening up further applications.

Overall, the goal is to learn how to design both compositions and process routes to yield the desired properties in materials without the need for extensive empirical experimental research. Evidence that this approach is working can be seen from the fact that the jet vane shown in figure 5a was developed in only about 6 months once the basic properties – processing – microstructure relationships had been established.

Future work for the group is planned to see further progress being made on the development of a whole suite of materials capable of withstanding different extreme environments, from the 1500^{o}C desired for jet engine materials to the 3000^{o}C for rockets, as well as work on the additive manufacturing of ceramic-based materials. Work on both approaches has already started and good progress has been made. An interesting 'side-line' has been the development of processes for use with extra-terrestrial materials using lunar and Martian regoliths; the aim being to assist in making progress towards the ability to create buildings and habitable spaces on these bodies without the need to take everything from earth.

Figures

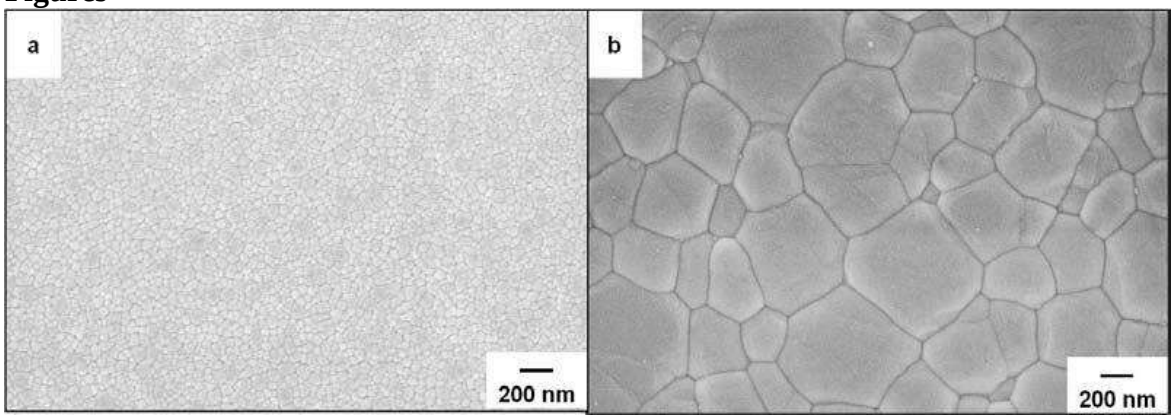


Figure 1: Microstructures of nanostructured and conventional grain size yttria stabilised zirconia at the same magnification.

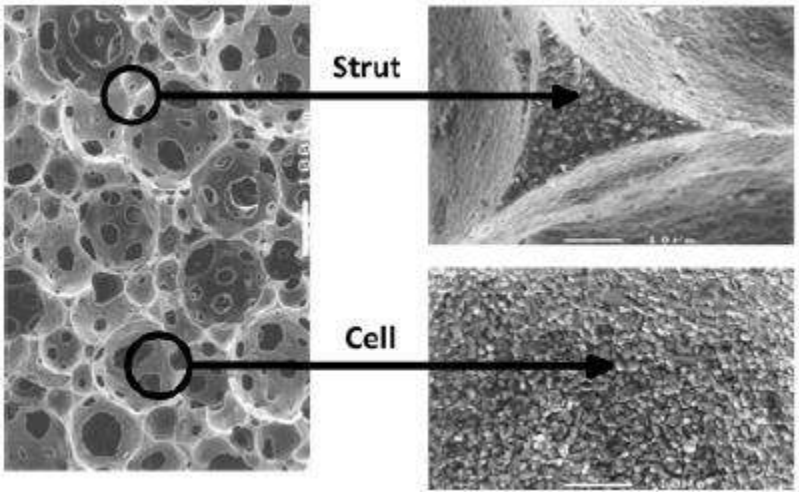


Figure 2: Typical micrograph of a 30% dense alumina foam.

Figure 3: A small selection of alumina ceramic foam product shapes.

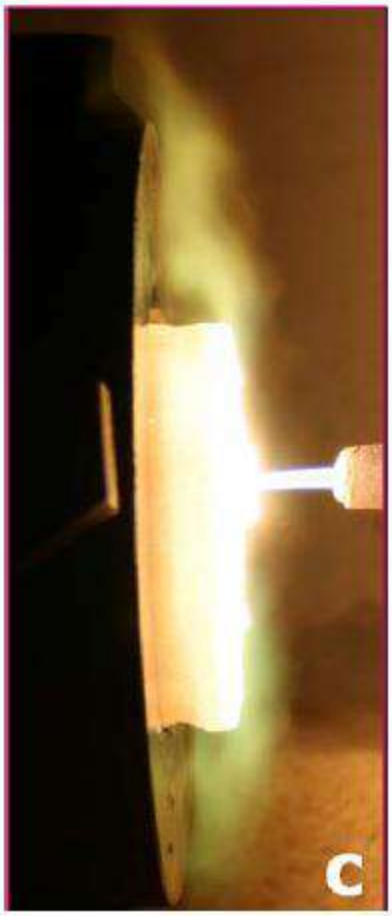


Figure 4: A Cf-HfB_2 composite being tested using an oxyacetylene torch.

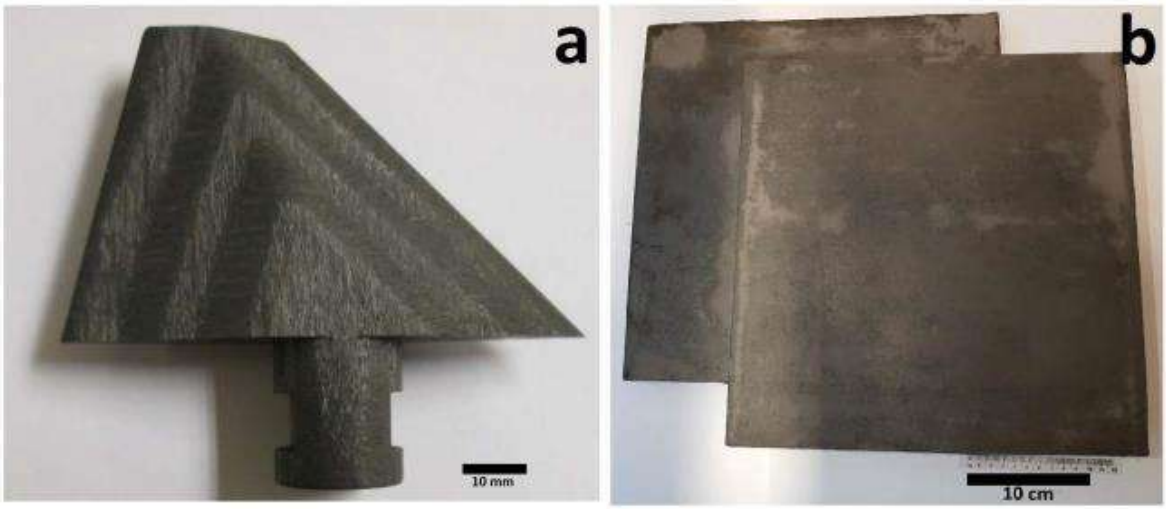


Figure 5: (a) A jet vane made as an MBDA demonstrator part and (b) DSTL large panels manufactured with Cf-HfB_2 composite.

Look into the Microscopic World of Pipeline Corrosion for Innovation of its Management

by Y. Frank Cheng, Member of EUAS

Short Biography

Professor and Canada Research Chair in Pipeline Engineering, University of Calgary
An internationally recognized authority in Corrosion Science and Engineering of Oil/Gas and Pipeline Systems

Education

2000 *Ph.D. in Materials Engineering, University of Alberta, Canada*
1993 *M.Sc. in Corrosion, Institute of Metal Research, Chinese Academy of Sciences*
1990 *B.Sc. in Corrosion, Hunan University, China*

Employment

2012 – present	*Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada*
2009 – 2012	*Associate Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada*
2005 – 2009	*Assistant Professor, Canada Research Chair in Pipeline Engineering University of Calgary, Canada*
2002 – 2005	*Research Scientist, Centre for Nuclear Energy Research, University of New Brunswick, Canada*
2000 – 2002	*NSERC Industrial Research Fellow, NOVA Research and Technology Center, Canada*
1993 – 1996	*Research Assistant, Institute of Metal Research, Chinese Academy of Sciences, China*

Awards

2018 *Member of EU Academy of Sciences (EUAS)*
2018 *Changjiang Scholar, Ministry of Education, China*
2018 *Research Achievement Award, University of Calgary, Canada*
2018 *Teaching Achievement Award, University of Calgary, Canada*
2018 *Supervision Excellence Award, China Scholarship Council (CSC)*
2017 *Metal Chemistry Award, Canadian Metallurgy and Materials Society (MetSoc)*
2017 *Research Achievement Award, University of Calgary, Canada*
2017 *Teaching Achievement Award, University of Calgary, Canada*
2017 *Supervision Excellence Award, China Scholarship Council (CSC)*
2016 *Fellow, NACE International, the Corrosion Society, U.S.A.*
2015 *Shi Chang-Xu Award, Chinese Society for Corrosion and Protection*
2014 *Herbert H. Uhlig Award, NACE International, the Corrosion Society, U.S.A.*
2010 *Engineering Student Society Teaching Excellence Award, University of Calgary, Canada*
2010 *Canada Research Chair in Pipeline Engineering (renewal)*
2009 *Research Excellence Award, University of Calgary, Canada*

2005 Canada Research Chair in Pipeline Engineering
2000 Industrial Research Fellowship, Natural Science and Engineering Research Council of Canada

Key Professional Service and Appointments

2018 Chair of Technical Committee on Materials Technology, Canadian Society of Mechanical Engineering
2018 Associate Editor of Transactions of Canadian Society for Mechanical Engineering
2017 Fellow Member, Task Force for Spotlight on Corrosion, NACE International
2017 Overseas Review and Evaluation Expert, Chinese Academy of Science
2017 Member of International Committee on Review and Evaluation of Chemistry Program of Huazhong University of Science and Technology, China
2015 Country (Canada) Leader, NACE International IMPACT Global Study Program
2015 Member of International Scientific Advisory Board, Institute of Oceanology, Chinese Academy of Science
2014 Chair of NACE International Task Group "Testing of Nonshielding Property of Pipeline Coatings to Cathodic Protection"
2014 Treasurer of NACE Foundation of Canada
2014 Chair of NSERC Site Visit and Review Committee for Industrial Research Chair in Nuclear Materials Corrosion
2013 Member of Canadian Crude Transmission Pipeline Roadmap Steering Committee
2012 Member of U.S. National Academy of Sciences (NAS) Committee on Pipeline Transportation of Diluted Bitumen
2009 Member of Board of Directors of Canadian Fracture Research Corporation
2008 Theme Editor in Pipeline Engineering of Encyclopedia of Life Support System (EOLSS) developed under the auspices of UNESCO

Pipelines are regarded as “energy highway” to transport oil, natural gas and petrochemical products from the production sites and processing plants to the markets and consumers. While pipelines have implemented their functions both effectively and efficiently over a half century, they are being prominent in debates on appropriate balances between economic, environmental and social goals the worldwide range in recent years. The primary spotlight exposing pipelines to relevant stackholders and the public is their safety and, once failed, the resulting impacts to environment, ecology and the community.

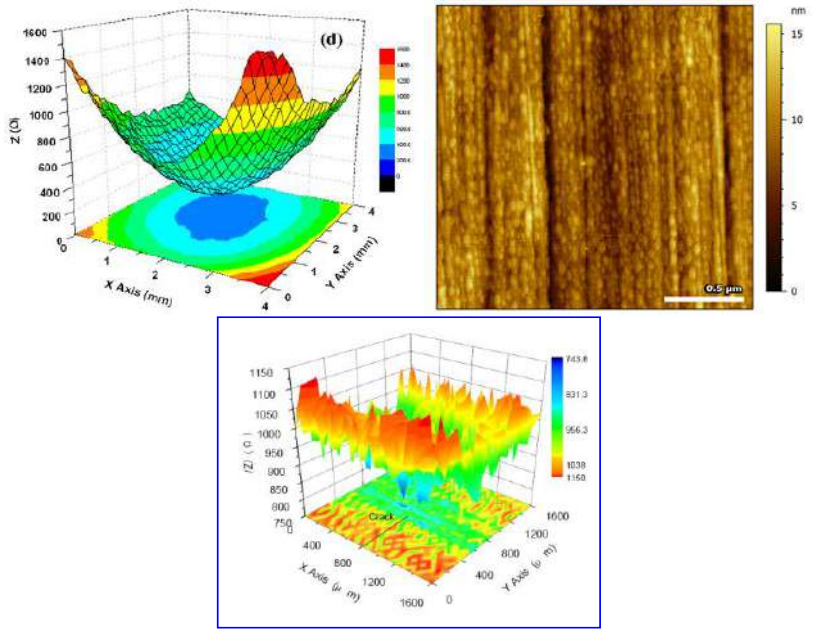
Among various mechanisms causing pipeline failures, corrosion has been identified as the most important one, as demonstrated by statistics in Canada, the United States and the world. Pipeline corrosion is a complex phenomenon, and the complexity arises as a result of multiple reactions and processes occurring simultaneously, which in turn, are very specific to the interactions of pipeline steels, environmental conditions and mechanical stresses the pipelines are exposed to.

The goal of Dr. Cheng’s research is to advance our understanding to the fundamentals of pipeline corrosion at a microscopic scale and thus at a more mechanistic level, and to improve pipeline integrity by technology innovation in modeling, prediction, prevention and monitoring of pipeline failures.

Metallurgical micro-electrochemistry of pipeline corrosion

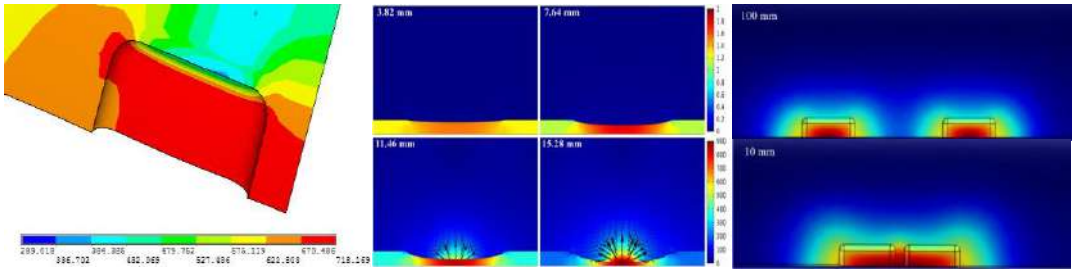
Corrosion of metals is electrochemical in nature. While various electrochemical techniques enable fundamental understanding of the corrosion phenomenon, they suffer from an essential limitation, i.e., the electrochemical measurement techniques provide macroscopic, averaged information of the metallic information. Actually, the failures of the majority of metallic structure in practice are not resulted from uniform corrosion, but localized corrosion, such as pitting, cracking, etc., which usually occurs at spatial

dimension of microns. Dr. Cheng is the pioneer researcher in the world to use micro- and nano-electrochemical techniques to "visualize" the pipeline corrosion at a microscopic level and advance the corrosion understanding at a more mechanistic level, contributing to the knowledge base of metallic corrosion. Dr. Cheng developed a Metallurgical Micro-Electrochemistry concept, characterizing the local electrochemical activities of varied micron-scaled metallurgical features in environments and determining the mechanisms for initiation of corrosion pits in the steels. He is the first researcher to categorize the metallurgical inclusions into "anodic" and "cathodic" types. Moreover, Dr. Cheng characterized the electrochemical activity and the preferential dissolution of nano-scaled features in the environments, leading this area in the world. He also modeled and determined quantitatively, at its first time, the contributions of stress and hydrogen, as well as their synergism, to growth rate of stress corrosion cracks on pipelines in near-neutral pH electrolytes. All of them contribute to a strong science base of pipeline corrosion.



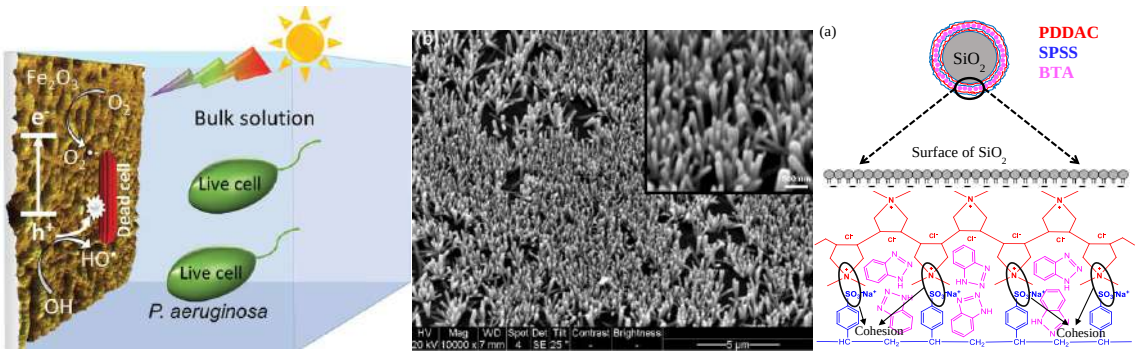
Mechano-electrochemical interaction at corrosion defects on pipelines

Pipelines are pressurized infrastructure, and pipeline corrosion occurs under a complex stressing condition. In addition to hoop stress resulted from the internal operating pressure, the pipelines also experience axial stress due to ground movement and local bending. Dr. Cheng is the first researcher to extend the mechano-electrochemical interaction theory in pipeline corrosion area, and improves the theory to quantify the effects of elastic and plastic deformations on the steel corrosion by modeling the multi-physics field coupling effect on pipelines. His findings confirmed the essential link of mechanics, metallurgy and electrochemistry in pipeline corrosion, advancing our knowledge base in stress corrosion of metals. At the same time, the research outcomes provide a solid theoretical foundation for improved pipeline integrity management.



Advanced materials technology for corrosion prevention

The emergence and development of advanced materials technology revolutionize the conventional engineering research, including corrosion science and engineering. Specifically, nanopatterning of metals can achieve a surface nanostructure with a low surface energy, enabling multiple novel functions. Dr. Cheng developed a novel technique to nanopattern carbon steels, the most extensively used engineering materials, to achieve a remarkable anti-biofouling performance. He improved the technique using the photo-catalytic ability of the nanofilms to further enhance the surface anti-biofouling. In addition to killing bacteria on the filmed steels, Dr. Cheng modified the surface nanofilms to make them possess self-cleaning ability for removal of dead bacterial cells. At the same time, Dr. Cheng developed novel nanocomposite photo-electrodes to enable both generation of photoelectrons for cathodic protection (CP) and self-storage of the photoelectrons for functionalization of the photoelectrochemical CP in the absence of light illumination. The technique utilizes the solar energy to supple the power for corrosion prevention of infrastructures by CP, while maintaining the environmental conservation by reduction of power consumption, especially the fossil energy. Dr. Cheng developed a smart coating technique to enable uniform distribution of inhibitor-stored nanocontainers in epoxy coatings, and self-releasing of the pre-loaded inhibitors in response to generation of corrosive environments at the coating failures. He also determined the inhibitor-releasing kinetics to predict the effective service life for corrosion inhibition of the coatings, laying a sound foundation for industrialization of the product for practical application.



Oncogenic Signal Transduction Pathways

by Jonathan Chernoff, Member EUAS

Short Biography

Education

1974-1978	*Yale College, BA, Molecular Biophysics/Biochemistry*
1978-1984	*Mount Sinai School of Medicine, MD/PhD Biochemistry*

Appointments

1984 - 1987	*Resident, Department of Internal Medicine, University Health Center of Pittsburgh, Pittsburgh, PA*
1987 - 1988	*Clinical Fellow, Department of Medical Oncology, The Johns Hopkins Oncology Center, Baltimore, MD*
1988 - 1990	*Clinical Fellow, Hematology/Oncology Department, Beth Israel Hospital, Boston, MA*
1988 - 1991	*Postdoctoral Fellow, Department of Cellular and Developmental Biology, Harvard University, Cambridge, MA*
1991 - 1997	*Assistant Professor, Fox Chase Cancer Center, Philadelphia, PA*
1997 - 2002	*Associate Professor, Fox Chase Cancer Center, Philadelphia, PA*
1997 -	*Program Leader, Cancer Biology Program, Fox Chase Cancer Center, Philadelphia, PA*
2002 - 2008	*Professor, Fox Chase Cancer Center, Philadelphia, PA*
2008 - 2010	*Vice President, Deputy Scientific Director, Stanley P. Reimann Chair in Oncology Research, Fox Chase Cancer Center, Philadelphia, PA*
2010 -	*Chief Scientific Officer and Cancer Center Deputy Director, Stanley P. Reimann Chair in Oncology Research, Fox Chase Cancer Center, Philadelphia, PA*

Other Experience and Professional Memberships

2000 - 2005	*Editor, Journal of Biological Chemistry*
2006 -	*Editor, Molecular Biology of the Cell*
2006 -	*Editor, Faculty of 1000*
2015 -	*Editor, Cancer Biological Therapy*

Honors

1978	*B.S. cum laude, Yale University*
1992	*Traveling Fellow Award, Pfizer*
1997	*Scholar Award, Leukemia Society of America*
2007	*Dozor Lecturer, Ben-Gurion University, Israel*
2010	*Scientific Research Award, American Cancer Society, Southeast PA Division*
2013	*PDDI Drug Discovery Award, Pennsylvania Drug Discovery Institute*
2016	*Senior Faculty Award, 4th Annual Temple Translation Science Symposium*
2016	*Interurban Clinical Club*
2017	*Fellow, American Association for the Advancement of Science*

Overview: Contribution to Science

Peer-reviewed publications: *~185`; H index = 72. 40 of my papers have been cited more than 100 times.*

I have devoted my research career to understanding how cells receive and interpret signals, and how this process in corrupted in cancer. In particular, I have focused on the regulation of signal transduction by phosphorylation. My overarching goal is to understanding of mechanisms underlying how signal transduction pathways are rewired in cancer, and their implications for the development, spread, and resistance of solid tumors to therapy.

My group has made important discoveries in three signaling pathways: Rho-family small GTPases, Hippo, and Insulin signaling, through discoveries and subsequent work on the STE20 kinases Pak and Mst, and the protein tyrosine phosphatase PTP1B, respectively, as detailed below. I have been funded without pause by the NIH (NCI and/or GM) since 1992, and during this time, our group has developed broad expertise in molecular biology, biochemistry, cell biology, proteomics, and mouse models of cancer.

Despite my substantial administrative responsibilities my group remains highly productive: since 2008, we have published more than 80 peer reviewed papers, including publications in Nature, Developmental Cell, Blood, Chemistry & Biology, PNAS, and ELife. Importantly, I also have a key role in education and mentoring, in that I have mentored dozens of postdoctoral fellows and graduate students over the years, as well as serving as Principle Investigator on Fox Chase's T32 training grant and its American Cancer Society Institutional Research Grant.

1. Protein Tyrosine Phosphatases (PTPs). My early work focused on the characterization and cloning of PTPs, with the idea that these might represent tumor suppressors. At that time, Ray Erikson and others had identified PTKs as oncogenes, but no PTPs had been described. As a graduate student, I found that several classical protein phosphatases, including prostatic acid phosphatase and PP2A, contained a latent ability to act as PTPs. Later, I isolated "pure" PTPs and then, as a postdoctoral fellow, was the first to clone the cDNA for the most abundant of these enzymes, PTP1B. While we found that PTP1B suppressed certain proliferative and motility signals, we also found that PTP1B could, in some cases, act to promote carcinogenesis, via activating c-Src. We later found that PTP1B was regulated by sumoylation, one of the first instances of regulation of an extra-nuclear protein by this mechanism.

a. **Chernoff, J.,** Schievella, A.G., Jost, C.J., Erikson, R.L. and Neel, B.G. Cloning of the cDNA of a major human protein-tyrosine-phosphatase. *Proc. Natl. Acad. Sci. USA.* **87**:2735-2739, 1990. (217 cites)
b. Liu, F., Sells, M.A., and **Chernoff, J**. Protein tyrosine phosphatase 1B negatively regulates integrin signaling. *Curr. Biol.* **8**:173-176, 1998. (142 cites)
c. Dadke, S., Cotteret, S., Yip, S.-C., Jaffer, Z.M., Haj, F., Ivanov A., Rauscher III, F., Shuai, K., Ng, T., Neel, B.G., and **Chernoff, J.** Regulation of Protein-Tyrosine Phosphatase (PTP) 1B by sumoylation. *Nat. Cell Biol.* **9**:80-85, 2007. (95 cites)
d. Arias-Romero, L.E., Saha, S., Villamar, O., Yip, S.-C., Ethier, S.P., Zhang, Z-Y., and **Chernoff, J.** Activation of Src by Protein Tyrosine Phosphatase (PTP)1B is required for ErbB2 transformation of breast epithelial cells. *Cancer Res.* **69**:4582-4588, 2009. (63 cites) PMC2692630

2. Mammalian Ste20-like kinases (Msts): Shortly after starting my independent career, I used a PCR-based screen to identify gene fragments for protein kinases that might act upstream of ERK. From this screen I obtained Mst1 and Mst2 as well as Pak1 and Pak2. We cloned and named Mst1 and Mst2 and were the first to demonstrate that they acted as dimers, which proved key to understanding their mechanism of regulation and downstream functions. With the Krebs' and Allis' labs, we were the first to demonstrate the apoptotic functions of the Mst proteins. We are currently exploring how Ras proteins regulate Mst activity in cancer (Rawat *et a*l., revised ms submitted))
   a. Creasy, C.L. and **Chernoff, J**. Cloning and characterization of a human protein kinase with homology to Ste20. *J. Biol. Chem.* **270**:21695-21700, 1995. (186 cites)
   b. Creasy, C.L., Ambrose, D.M., and **Chernoff, J**. The human Ste20-like kinase, Mst1, dimerizes and contains an inhibitory domain. *J. Biol. Chem.* 271:21049-21053, 1996. (145 cites)
   c. Cheung, W.L., Ajiro, K., Samejima, K., Kloc, M., Cheung, P., Mizzen, C.A., Beeser, A., Etkin, L.D., **Chernoff, J**., Earnshaw, W.C., and Allis, C.D. Apoptosis in vertebrates is characterized by phosphorylation of histone H2B mediated by Mammalian Sterile Twenty kinase *Cell*, **113**:507–517, 2003. (364 cites)
   d. Rawat, S.J., Araiza-Olivera, D., Arias-Romero, L.E., Villamar-Cruz, O., Prudnikova, T.Y., Roder, H., and **Chernoff, J**. H-ras inhibits the hippo pathway by promoting Mst1/Mst2 heterodimerization. *Curr. Biol.* **26**:1556–1563, 2016

3. p21-activated kinases - basic biology: We were among the first to identify these kinases, and the first to show that Pak alters the cytoskeleton and cell motility. We also delineated the basic signaling pathways that link Paks to cell proliferation and survival pathways. Our papers and reviews in this area are among the most highly cited in the field.
   a. Sells, M.A., Knaus, U.G., Bagrodia, S., Ambrose, D., Bokoch, G.M., **Chernoff, J.**Human p21-activated kinases (Paks) regulate actin reorganization in mammalian cells. *Curr. Biol.* **7**:202-210, 1997. (639 cites)
   b. Sells, M.A., Boyd, J.T., **Chernoff, J.** Human p21-activated kinase (Pak1) regulates motility of mammalian fibroblasts. *J. Cell. Biol.* **145**:837-849, 1999. (374 cites)

c. McDaniel, A.S., Allen, J.D., Park, S.J., Jaffer, Z.M., Michels, E.G., Burgin, S.J., Chen, S., Bessler, W.K., Hofmann, C., Ingram, D.A., **Chernoff, J.***, Clapp, D.W. Pak1 regulates multiple c-Kit mediated Ras-MAPK gain-in-function phenotypes in Nf1(+/-) mast cells. *Blood* **112**:4646-4654, 2008. (*co-senior author) PMC2597131 (74 cites).

d. Kelly, M.L., Astsaturov, A., Rhodes, J., and **Chernoff, J**. A Pak1/Erk signaling circuit acts through Gata6 to regulate cardiovascular development in zebrafish. *Dev. Cell* **29**:350-9, 2014. PMC4073496.

4. p21-activated kinases – role in cancer: We made the first mouse knock-out models of Pak1 and Pak2, and used that to show that Pak1 is essential for K-ras-mediated carcinogenesis. We also (with Jeff Peterson) identified the specific first specific small molecule inhibitor of group I Paks (IPA3), which remains in wide use today. Finally, with the Testa lab, we linked Pak signaling to the NF2 (Merlin) tumor suppressor), setting the stage for rational development of therapeutics in this disorder.

   a. Xiao, G.H., Beeser, A., **Chernoff, J**. and Testa, J.R. Pak links Rac/Cdc42 signaling to Merlin *J. Biol. Chem.* **277**: 883-886, 2002. (223 cites)

   b. Deacon, S.W., Beeser, A., Fukui, J.A., Rennefahrt, U.E.E., Myers, C., **Chernoff, J**., and Peterson, J. An isoform-selective, small-molecule inhibitor targets the autoregulatory mechanism of p21-activated kinase. *Chem. Biol.*, **15**:322-331, 2008. (Deacon and Beeser, co-first authors). (150 cites) PMC4353635

   c. Chow, H.Y., Jubb, A.M., Koch, J.N., Jaffer, Z.M., Stepanova, D., Campbell, D.A., Duron, S. G., O'Farrell, M., Cai, K.Q., Klein-Szanto, A.J., Gutkind, J.S., Hoeflich, K.P., and **Chernoff, J**. p21-activated kinase 1 is required for efficient tumor formation and progression in a Ras-mediated skin cancer model. *Cancer Res.* **72**:5966-75, 2012. PMC3500416

   d. Arias-Romero, L.E., Villamar-Cruz O., Huang, M., Hoeflich, K.P., **Chernoff, J.** Pak1 Kinase Links ErbB2 to β-Catenin in Transformation of Breast Epithelial Cells. *Cancer Res.* **73**:3671-82, 2013. PMC3687032

Complete List of Published Work in My Bibliography:
http://www.ncbi.nlm.nih.gov/myncbi/jonathan.chernoff.1/bibliography/40856644/public/?sort=date&direction=ascending

Innovations in Flat Panel Technolgies

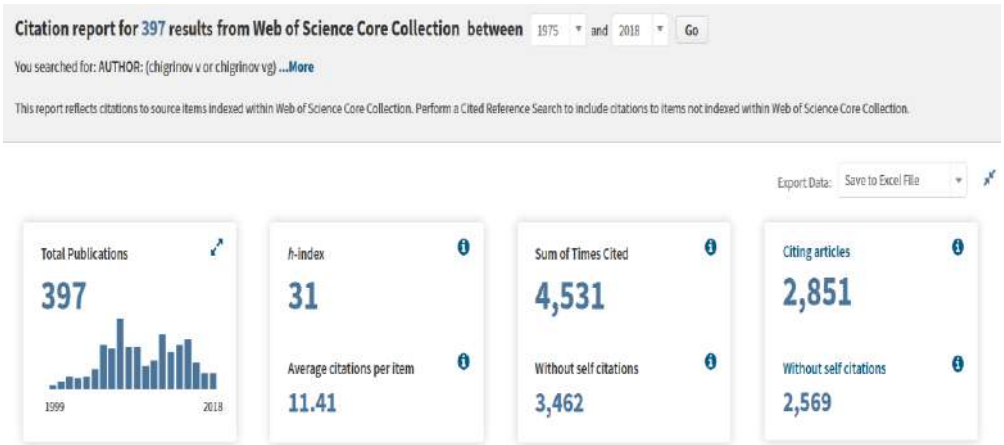
by Vladimir Chigrinov, Member EUAS

Short Biography

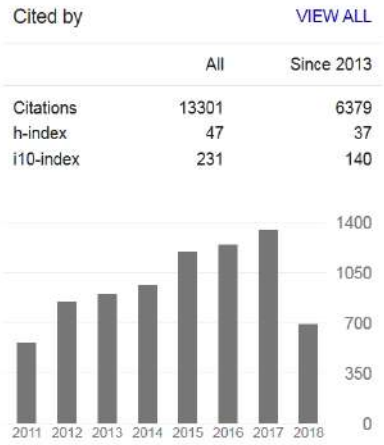
Professor Vladimir G. Chigrinov is Professor of Hong Kong University of Science and Technology since 1999. He is an Expert in Flat Panel Technology in Russia, recognized by the World Technology Evaluation Centre, 1994, and SID Fellow since 2008. He is an author of 6 books, 25 reviews and book chapters, about 283 journal papers, more than 634 Conference presentations, and 112 patents and patent applications including 29 US patents in the field of liquid crystals since 1974. He got Excellent Research Award of HKUST School of Engineering in 2012. He obtained Gold Medal and The Best Award in the Invention & Innovation Awards 2014 held at the Malaysia Technology Expo (MTE) 2014, which was hosted in Kuala Lumpur, Malaysia, on 20-22 Feb 2014. He is a Member of EU Academy of Sciences (EUAS) since July 2017. He got a 2018 Slottow Owaki Prize of SID.

The paper of M.Schadt, K.Schmitt, V.Kozenkov, V.Chigrinov, Surface-induced parallel alignment of liquid crystals by linearly polymerized photopolymers, Jap. J.Appl. Phys. P.I., Vol.31, pp. 2155-2164 (1992) is number 4 among the most heavily-cited and have been influential papers published in JJAP since the first volume (1962) and have been selected from the various fields of applied physics by the JJAP Editorial Board.

Web of Science citation index



Google Scholar citation index



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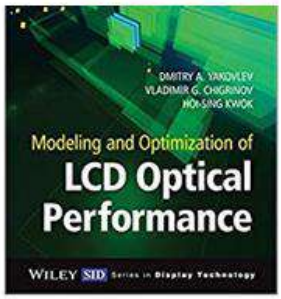
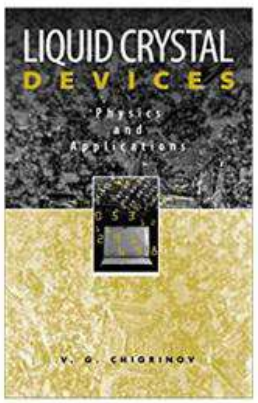
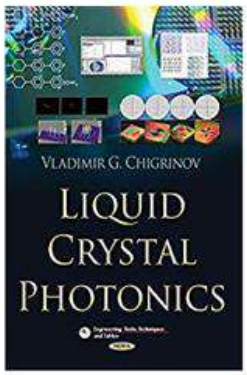
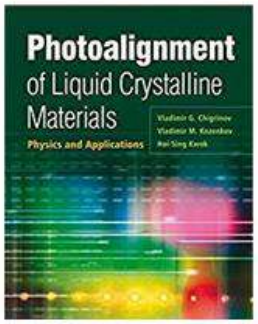
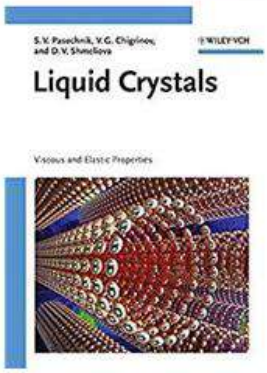
Books

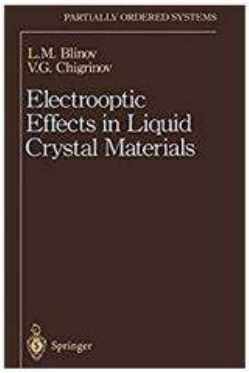












Russian Academy of Science, Institute of Crystallography, Russian Academy of Informatics and Electronics:

1.T.V. Korkishko, " Electrooptics of LC-surface interaction", Shubnikov Institute of Crystallography, Russian Academy of Sciences, PhD, 1987.
2. V. Shapovalov, " Flow effects in LC electrooptic phenomena", Moscow State University, PhD, 1987.
3.Yu.P.Panarin, "Bistability in thin layers of Ferroelectric Liquid Crystals", Russian Academy of Informatics and Electronics, PhD, 1993.
4. V.P.Vorflusev,"Electrooptics and Surface Interaction in Thin Layers of Ferroelectric LCs", Russian Academy of Informatics and Electronics, PhD, 1995.
5. G.V.Simonenko, "Computer Simulation of Electrooptical Effects in LCs", Russian Academy of Informatics and Electronics, PhD,1995.

Hong Kong University of Science and Technology:

1. Danding Huang, "Ferroelectric Liquid Crystal Display Photo-aligned by Azo-dye layers", August, 2004.
2. Anatoli Murauski, " Surface and liquid crystal interlayer interactions: characterizations and applications", July, 2007.
3. Xihua Li, "Bi and Multistable Ferroelectric Liquid Crystal Displays using Non-contacting Aligning Methods",February, 2008.
4. Xu Peizhi, "Electrooptical Modes in Nematic and Ferroelectric Liquid Crystals: Optimization for Display and Shutter Applications", September, 2008.
5. Alexander Muravski, " Liquid Crystal Devices for Display and Photonics Applications, based on Photoalignment Technology", September, 2008.
6. Fan Fan, Liquid Crystal Patterned Photoalignment: Methods and Applications, August, 2013.
7. Qi Guo, Fast electrooptical modes in ferroelectric liquid crystal and their applications, August, 2013.
8. WANG Xiaoqian, Novel Liquid Crystal Diffractive Lenses and Display, May, 2014.
9. Jiatong Sun, Liquid Crystal Power Saving Display: Optically Rewritable E-Paper and Its Applications, May, 2014.
10. Tao Du, Photo-Patterned thin film polarizer with close to 100% efficiency, December, 2014.
11. Ying Ma, Electrically Suppressed Helix Ferroelectric Liquid Crystals and Their Application, May 2015.
12. Alwin Ming Wai Tam, Liquid Crystals Pancharatnam-Berry Phase Devices: Fabrication and Applications, August 2016.

Awards

Senior Member of the Society for Information Display (SID) since 10.10.04.
SID Fellow since 15.01.08
The Research Excellence Award of SENG, HKUST, that recognizes the efforts of an outstanding faculty member with a proven record of research excellence, May 2012.
Gold Medal and The Best Award in the Invention & Innovation Awards 2014 held at the Malaysia Technology Expo (MTE) 2014, which was hosted in Kuala Lumpur, Malaysia, on 20-22 Feb 2014.
Member of EU Academy of Sciences (**EUAS**) of distinguished members worldwide since

July 2017.
2018 Slottow-Owaki Prize "For his educational efforts in the field of liquid-crystal devices, as evidenced by his teaching, supervision of graduate students, and prolific publications and conference presentations."

Recent publications

1.Chia-Ming Chang, Yi-Hsin Lin, Abhishek Kumar Srivastava, and Vladimir Grigorievich Chigrinov, An optical system via liquid crystal photonic devices for photobiomodulation, *Scientific Reports, | (2018) 8:4251, pp.1-10,* www.nature.com/scientificreports.
2. YUE SHI, YAN JUN LIU, FENG SONG, VLADIMIR G. CHIGRINOV, HOI-SING KWOK, MINGGANG HU, DAN LUO, AND XIAO WEI SUN, Photoalignment-induced two-dimensional liquid crystal polarization structure via multi-beam polarization interferometry, *Optics Express*, Vol. 26, No. 6, pp. 7683-7692 (2018).
3. Su Pan, Jacob Y. Ho, Vladimir G. Chigrinov, and Hoi Sing Kwok, Novel Photoalignment Method Based on Low-Molecular-Weight Azobenzene Dyes and Its Application for High-Dichroic-Ratio Polarizers, *ACS Appl. Mater. Interfaces* , Vol. 10, pp. 9032−9037 (2018).
4. L. Wang, J. Sun, H. Liu, V. G. Chigrinov & H. S. Kwok, Increasing the rewriting speed of ORW e- paper by electric field, *Liquid Crystals*, Vol. 45, No. 4, pp. 553–560 (2018).
5. Benjamin S.-Y. Ung, Xudong Liu, Edward P. J. Parrott, , Abhishek Kumar Srivastava, Hongkyu Park, Vladimir G. Chigrinov, and Emma Pickwell-MacPherson, Towards a Rapid Terahertz Liquid Crystal Phase Shifter: Terahertz In-Plane and Terahertz Out-Plane (TIP-TOP) Switching, *IEEE TRANSACTIONS ON TERAHERTZ SCIENCE AND TECHNOLOGY*, Vol. 8, N 2 , pp 209-214 (2018).

Mechanisms to Control Neurodegeneration & Neuronal Cell Death

by Ted Dawson, Member EUAS

Short Biography

Ted Dawson has dedicated his career to deciphering the mechanisms that control neurodegeneration and neuronal cell death. His most recent work has focused on the genetic pathways responsible for familial and acquired Parkinson's disease and poly (ADP-ribose) signaling.

Dawson attended Montana State University and received a B.S. in Premedicine in 1981 with highest honors. He received a M.D. and Ph.D in Pharmacology in 1986 from the University of Utah where he also completed an Internship in Internal Medicine. At the Hospital of the University of Pennsylvania, he completed a Neurology Residency in 1990. After postdoctoral training with Solomon H. Snyder and a clinical movement disorder fellowship at Johns Hopkins University School of Medicine, he joined the Departments of Neurology and Neuroscience in 1994 and became Professor in 2000. From 1996 to 2010 he was director of the Parkinson's Disease and Movement Disorder Center. He founded the Neuroregeneration Program in the Institute for Cell Engineering in 2002 and became the Scientific Director of the Institute for Cell Engineering in 2010 and its Executive Director in 2011. He is currently the Leonard and Madlyn Abramson Professor in Neurodegenerative Diseases and Director of the Institute for Cell Engineering.

Dawson's honors include the Derek Denny-Brown Young Neurological Scholar Award from the American Neurological Association, the Paul Beeson Physician Faculty Scholar Award, the Santiago Grisolia Medal Santiago Grisolia Medal, Thomson Reuters Highly Cited Researcher Award and Worlds' Most Influential Scientific Minds and the Javits Neuroscience Investigator Award. He was elected to the Association of American Physicians and is a Fellow of the American Association for the Advancement of Science, American Academy of Neurology and the American Heart Association. He is world-renowned for his novel contributions on the role of nitric oxide (NO) in neuronal injury and signaling and understanding the molecular basis of neurodegeneration in Parkinson's disease. He has published over 535 publications with an H-index of 151 (Google Scholar). He is one of the top five cited Neuroscientists in the last decade and is a 2014-15 Thomson Reuters Highly Cited Researcher.

He is a member of the Board of Directors for the Bachman-Strauss Dystonia and Parkinson Foundation and serves on the Medical Advisory Board of the Cure Progressive Supranuclear Palsy Foundation, the General Advisory Council (GAC) of the Parkinson's Disease Research Roadmap (PDRR) Initiative of the Milken Institute and a member of the Executive Scientific Advisory Board of Michael J. Fox Foundation for Parkinson's Research. He is a member of numerous editorial boards including the Journal of Clinical Investigation and Cell.

Research Summary

Many advances in the neurobiology of disease have stemmed from Dr. Dawson's identification of the mechanisms of neuronal cell death and the elucidation of the molecular mechanisms of neurodegeneration. His studies of NO led to major insights into the neurotransmitter functions of this gaseous messenger molecule. He pioneered the role of NO in neuronal injury in Parkinson's disease, stroke and excitotoxicity. He showed that NO derived from neuronal NO synthase and immunologic NO synthase leads to degeneration of dopamine neurons through cell autonomous and non-cell autonomous affects, respectively. Dawson elucidated the molecular mechanisms by which NO kills neurons through the actions of poly (ADP-ribose) (PAR) polymerase (PARP) and discovered a unique cell death pathway designated parthanatos, in which PAR functions as an intracellular signaling molecule that induces the release of apoptosis inducing factor (AIF) causing cell death via the recruitment of the nuclease, macrophage migration inhibitory factor (MIF). He showed that poly (ADP-ribose) glycohydrolase, which degrades PAR polymer is an endogenous inhibitor of parthanatos. In screens for neuroprotective proteins, he discovered another endogenous inhibitor of parthanatos, Iduna (RNF146), a first in class PAR-dependent E3 ligase. In the same screens, he also discovered Thorase, an AAA+ ATPase that regulates glutamate (AMPA) receptor trafficking and discovered that Thorase is an important regulator of synaptic plasticity, learning and memory. Botch was also discovered as in important inhibitor of Notch signaling via deglycination of Notch preventing Notch's intracellular processing at the level of the Golgi, playing an important role in neuronal development.

Dawson has also been at the forefront of research into the biology and pathobiology of the proteins and mutant proteins linked to Parkinson's disease. Dr. Dawson showed that parkin is a ubiquitin E3 ligase that is inactivated in patients with genetic mutations in parkin and that it is also inactivated in sporadic Parkinson's disease via *S*-nitrosylation and c-Abl tyrosine phosphorylation leading

to accumulation of pathogenic substrates. He discovered the parkin substrate, PARIS, which plays a key pathogenic role in PD pathogenesis by inhibiting mitochondrial biogenesis. He showed that DJ-1 is an atypical peroxidoxin-like peroxidase and that its absence in PD leads to mitochondrial dysfunction. He showed that mutations in LRRK2 cause PD through pathologic kinase activity leading to enhanced protein translation via the phosphorylation of the ribosomal protein s15 and that inhibiting LRRK2 is protective. His laboratory discovered that pathologic α-synuclein spreads in the nervous system via engagement with the lymphocyte-activation gene 3 (LAG3). These studies are providing major insights into understanding the pathogenesis of PD and stroke and are providing novel opportunities for therapies aimed at preventing the degenerative process of PD and other neurologic disorders.

Publications

Full publication list:
https://scholar.google.com/citations?hl=en&user=XNbJbbkAAAAJ

Epigenetics of Prostate Cancer Development

by William Nelson, Member EUAS

Short Biography

Dr. Nelson has served as the Marion I. Knott Professor of Oncology and Director of the Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins since 2008. He currently holds Professorships in Oncology, Medicine, Pharmacology, Pathology, Radiation Oncology, Urology, and Environmental Health Sciences. His laboratory discovered one of the first epigenetically-silenced genes in cancer, GSTP1, inactivated in nearly all prostate cancer cases. GSTP1 DNA methylation assays approved by the US Food and Drug Administration as adjuncts for prostate cancer diagnosis comprise the first epigenetic laboratory tests in common use. Dr. Nelson and colleagues also identified the major precursor to prostate cancer, 'proliferative inflammatory atrophy,' implicating recurrent injury and inflammation in the pathogenesis of the disease.

After earning a Bachelor's degree in Chemistry from Yale University in 1980, Dr. Nelson received a Doctor of Philosophy degree in Pharmacology and a Doctor of Medicine degree from the Johns Hopkins University School of Medicine in 1987. He completed Internship and Residency training in Internal Medicine in 1990, and Fellowship training in Medical Oncology in 1992, all at the Johns Hopkins Hospital. Dr. Nelson joined the Johns Hopkins faculty as an Assistant Professor in 1992 and rose through the ranks to Professor by 2002.

Dr. Nelson has authored some 240 journal articles, earning >31,500 citations with an h-index of 96; he has also written 25 book chapters and monographs. Outside of Johns Hopkins, Dr. Nelson is a recognized leader in cancer research, organizing national and international meetings in cancer health disparities, cancer prevention, and prostate cancer, serving on the Board of the V Foundation, as a Scientific Co-Chair for Stand Up 2 Cancer, on the Scientific Advisory Board for the Prostate Cancer Foundation, and as a Co-Chair of the National Cancer-Institute Translational Research Working Group. He was elected to the American Association of Physicians in 2014. Dr. Nelson is the Executive Editor of Cancer Today, a Senior Editor of Cancer Research, and on the Editorial Board of the Journal of Clinical Investigation. Owner of 10 issued patents, he is a co-founder of Digital Harmonics, a Board Member of Armis Biopharma, and an Advisory Board Member for Abbvie, Cepheid, Proquest Investments, and Fulcrum2020 Investments.

Epigenetic Gene Silencing During Human Prostatic Carcinogenesis

Somatic epigenetic alterations accompany the development of most human cancers, including prostate cancer [1-3]. These genome changes, which affect chromatin structure and function, are through mitosis, *providing a selective advantage for growth and survival*

during cancer pathogenesis. Epigenetic defects in cancer cells reported thus far include: *(i)* transcriptional silencing of caretaker genes and tumor suppressor genes, *(ii)* reactivation of embryonic genes, *(iii)* loss of imprinted gene partitioning into active and inactive alleles, *(iv)* redirection of transcription promoter use, *(v)* disordered microRNA gene expression, (vii) activation of retrotransposition, and *(viii)* increased genetic recombination at repeat elements. Dr. Nelson and his colleagues and collaborators have shown that epigenetic changes arise at the earliest recognizable steps of transformation in the prostate and persist through invasion, metastasis, and lethal progression [4,5]. Growing knowledge of the extent of epigenetic alterations in prostate cancer has created new opportunities for the discovery of biomarkers useful for screening, detection, diagnosis, staging, and risk stratification [3]. In addition, because epigenetic processes do not irreversibly change genome sequence, therapeutic modulation of the epigenome, using drugs that affect dynamic chromatin function has great promise as a rational approach to prostate prevention and treatment.

Epigenome states, established in normal cells during development, are maintained through somatic cell mitosis as a consequence of "marks" present in genomic DNA and in chromatin proteins. The major DNA mark is symmetric methylation of cytosine bases in the self-complementary nucleotide sequence CpG. Most CpG dinucleotides carry this mark; unmethylated CpGs, clustered into ~1 kb regions encompassing the transcription start sites of many genes, have been termed "CpG islands" [6]. Somatic changes in DNA methylation at CpG islands affect gene activity. Genes with unmethylated CGIs are competent for regulated transcription, responding to signaling cues by recruiting *trans*-activating factors that modify nucleosome and chromatin structure, using histone acetyltransferases (HATs) and histone methyltransferases (HMTs) to promote transcript synthesis by RNA polymerases. In contrast, genes with methylated CGIs tend to be incompetent for expression, tightly wound around nucleosomes in a repressive chromatin structure maintained by histone deacetylases (HDACs) and other enzymes. Thus, somatic increases in CpG island methylation have been associated with gene silencing and heterochromatinization, while somatic decreases in DNA methylation have been implicated in illegitimate gene activation, retrotransposition, and recombination.

Changes in DNA methylation marks, accompanied by epigenetic gene silencing, appear to be the earliest somatic genome changes yet recognized in human prostate cancer. The most studied gene affected by *de novo* methylation during prostatic carcinogenesis is *GSTP1*, which encodes an enzyme responsible for detoxifying electrophiles and oxidants, including those that threaten cell and genome damage [3,7]. Hypermethylation of *GSTP1* transcriptional regulatory sequences has been detected in more than 90% of prostate cancers in more than 50 independent analyses, far more frequently than any other known somatic gene defect [2]. Loss of GSTP1 function likely occurs at the initiation of prostatic carcinogenesis, with *GSTP1* hypermethylation evident in some 5-10% of proliferative inflammatory atrophy (PIA) lesions, the earliest prostate cancer precursors, and in more than 70% of prostatic intraepithelial neoplasia (PIN) lesions [8,9]. Human prostate cancer cells devoid of GSTP1 tend to activate heterocyclic amine carcinogens, such as those found in overcooked meats, to mutagenic species [10]. Perhaps, *GSTP1* silencing early during the pathogenesis of PCA, with the resultant loss of enzymatic protection against reactive chemical species, may offer an explanation for the well-known sensitivity of human prostatic carcinogenesis to dietary and lifestyle habits [10-12]. In support of this notion, mice carrying disrupted *Gstp1/2* genes are more prone to develop skin tumors upon exposure to a topical carcinogen than wild-type mice [13]. Inadequate GSTP1 function also alters PCA cell responses to oxidant damage, leading to oxidation "tolerance" [14].

Chronic or Recurrent Prostate Inflammation as the Cause of Human Prostate Cancer

Both prostate cancer and prostatic inflammation have reached epidemic proportions among men in the United States (US) and developed world [11]. A diverse collection of etiologic factors, ranging from infectious agents to estrogenic hormones to dietary carcinogens, link damage to the prostate epithelium and prostate inflammation [15]. In an inflamed milieu, stressed prostate cells appear prone to neoplastic transformation. The transformed cells, in turn, can progress to invasive prostate cancer that grows uncontrollably, disseminates throughout the body, and threatens life. The pathogenesis of prostate cancer is accompanied by genetic and epigenetic alterations [11]. Although the precise mechanism(s) by which such defects arise during prostatic carcinogenesis have not been fully elucidated, accumulating data indicate that chronic inflammation constitutes a major threat to prostate cell genome and epigenome integrity, likely corrupting normal gene function that throughout the natural history of the disease.

Some sort of inflammation is ubiquitous in prostate tissues in the developed world where prostate cancer is common [16]. In the US, symptomatic prostatitis afflicts 10% or more of men, prompting at least 2 million physician visits each year. Asymptomatic prostatitis, usually detected by prostate biopsy, at radical prostatectomy, or at autopsy, is even more common. Asymptomatic prostatitis usually involves the peripheral zone of the prostate, where prostate cancers arise, further linking the two conditions. By disrupting the barrier function of the prostate epithelium, inflammatory processes tend to increase the serum prostate-specific antigen (PSA) in asymptomatic men, triggering prostate biopsy to search for early prostate cancer. For this reason, associations of prostate inflammation and prostate cancer have historically been difficult to study: if inflammation is a driver of prostate biopsies it will tend to be innately correlated with prostate cancer diagnoses. Nevertheless, despite this potential source of bias, a consistent association between prostatitis and prostate cancer has been reported in epidemiological analyses [17]. Men who participated in the Prostate Cancer Prevention Trial (PCPT) and the Selenium and Vitamin E Cancer Prevention Trial (SELECT) underwent prostate biopsies regardless of serum PSA values. A recent study of men who were on the placebo arms of both studies revealed that the odds of developing prostate cancer on the second prostate biopsy increased strikingly for men with extensive inflammation in benign prostate tissues an average of 5.9 years earlier [18].

The global prostate cancer epidemic has been attributed to dietary habits or other features of life in the developed world. The key mechanistic feature that links such exposures to prostate cancer may be damage to the prostate epithelium, which can both elicit an inflammatory response and perpetuate a chronic inflammatory state. Such exposures may include dietary heterocyclic amine carcinogens, estrogens, infections, urine reflux, and ischemia [15]. Prostate epithelial damage leads to focal epithelial atrophy, where prostate cells fail to fully differentiate, instead activating cellular stress response pathways [19,20]. One type of focal atrophy lesion, termed *proliferative inflammatory atrophy* (PIA), appears to be the earliest precursor to prostatic intraepithelial neoplasia (PIN) and to prostate cancer. In PIA lesions, epithelial stress leads to both regenerative epithelial cell proliferation and inflammation, suggesting a pathogenesis similar to many other epithelial cancer precursor conditions, including hepatitis/cirrhosis, atrophic gastritis, etc. The evidence implicating PIA in the pathogenesis of prostate cancer includes: *(i)* the emergence of somatic epigenome defects in rare PIA lesions that are also seen in PIN and in prostatic carcinoma, *(ii)* the close proximity of PIA lesions to PIN and to prostatic carcinoma, and *(iii)* and the appearance of PIA lesions in advance of PIN and of prostatic carcinoma in

exposure-driven mouse and rat models of prostatic carcinogenesis, including those associated with estrogens and with heterocyclic amine carcinogens [15].

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A Meshless-Stochastic Approach for Modeling Particulate Transport

by Darrell Pepper, Member EUAS

Short Biography

Darrell Pepper is Professor of Mechanical Engineering and former Director of the Nevada Center for Advanced Computational Methods (NCACM), which he founded in 1996, at the University of Nevada Las Vegas (UNLV). He was appointed Distinguished Visiting Professor at the US Air Force Academy from 2011-2013. Dr. Pepper served as Department Chair of Mechanical Engineering, as well as Interim Dean of the College of Engineering at UNLV, and was a Congressional Fellow working for Senator Feinstein in Washington, DC where he handled science, aerospace, and engineering issues. He obtained his B.S.M.E., M.S.A.E., and Ph.D. degrees from the University of Missouri – Rolla (now MS&T). Prior to his arrival at UNLV in 1992, Dr. Pepper held various technical and managerial positions with Dupont at the Savannah River Site in Aiken, SC. He served as Chief Scientist for the Marquardt Company in Van Nuys, CA, where he worked on the National Aerospace Plane program, and was CEO of a company he co-founded in southern California. He has given briefings to Congress and to several Presidential Science Advisors on modeling issues. Dr. Pepper has published over 350 technical papers on fluid dynamics, heat transfer, and environmental transport topics, including six textbooks on numerical modeling. He was a recipient of the 1996 Barrick Distinguished Scholar Award from UNLV, and the 1996 and 2011 Distinguished Research Award from the College of Engineering. He served as a member of the Baldrige Board of Examiners and was appointed a Commissioner to the ABET Engineering Accreditation Board in 2008. In 2008, he was awarded the Eric Reissner medal by the ICCES, the Harry Reid Silver State Research Award in 2010, the AIAA Distinguished Service Award in 2011, and the AIAA Energy Systems Award in 2012. He received the Lifetime Achievement Award from ICCES in 2015. He served on the Board of Directors of ABET from 2013-2015, and the Board of Delegates from 2015-2016. He has served as an ABET PEV Support Facilitator (trainer) since 2010.

Darrell W. Pepper is a researcher and educator in the areas of fluid dynamics, heat transfer, species transport, renewable energy and high-speed propulsion systems, and computational methods including finite elements, boundary elements, and meshless methods [1]. Dr. Pepper has published numerous technical papers on fluid dynamics, heat transfer, and environmental transport topics, including a series of textbooks on the finite element method, indoor air pollution modeling, and numerical modeling. He has received many awards, including the AIAA Sustained Service

Award, the AIAA Energy Systems Award, and the state of Nevada's top research award. In 2015, he was recognized internationally by ICCES for his lifetime achievements in environmental transport and fluid mechanics. He was the founder of the ASME K-20 Computational Heat Transfer Committee, an ASME Congressional Fellow where he served as senior legislative staff for US Senator Dianne Feinstein in Washington, DC, served as Deputy Chair of the ASME Committee for Research and Technology, and was a member of the ASME Board of Government Relations. He has served as an ABET Program Evaluator since 1994, and was an ABET EAC Commissioner, Member of the Board of Directors and Delegates, and a trainer for new accreditation program evaluators. The following describes his current research efforts in the use of meshless methods.

Current Research

1. Overview

A meshless-stochastic approach for modeling particulate transport is being used to simulate indoor particulate transport within buildings and rooms that can be displayed on mobile devices in real time. The approach utilizes the advantages of the meshless method by distributing collocation points and different order localized radial basis functions (RBFs) according to the computational domain and evolving numerical solution. This numerical scheme has been shown to yield fast convergence and high accuracy and has significant promise for providing valuable insight into aerosol and particulate transport physics as well as the ability to yield quick forecasts for remedial or preventive actions associated with indoor contamination [2-6].

Mesh-free methods with radial basis functions (RBF) have the following advantages:

(1) require neither domain nor boundary discretization;
(2) domain integration is not required;
(3) converge exponentially for smooth boundary shape and boundary data;
(4) insensitive to multiple dimensions and thus attractive to high dimensional problems;
(5) implementation and coding are very easy

In this research, the meshless method employing localized RBFs is coupled with stochastic particle transport. By coupling the meshless method with a stochastic Lagrangian particle technique, particulate transport traces can be quickly and accurately simulated and graphically displayed. The model includes the ability to access CAD drawings of a building; this permits quick assessment of a domain model of offices on a floor, including ventilation pathways. The hybrid numerical model is particularly appealing for evaluating particulate transport status as well as for risk assessment with emergency responders.

Collaboration is underway with other researchers to create a real-time capability for displaying computational results on tablets and handheld mobile devices using the meshless method. The ease with which one can employ meshless methods is remarkable and shows that a numerical technique does not need to become difficult or complex to be good. The coupling of the model with real-time sensors will ultimately lead to smart rooms and facilities that could respond instantly to the presence of hazardous substances and alter HVAC and air flows to permit safe evacuation. This was made apparent when experiencing ricin and anthrax threats while working in the U.S. Senate Hart and Dirkson Buildings in 2004.

2. Background

Indoor air pollution problems pose serious challenges to human health. Most people spend over 90 percent of their time indoors - at home, at work, or traveling in a vehicle. Researchers have

pointed out that exposure to indoor air pollution – emission of pollutants, their accumulation due to poor ventilation, and air exchange -- can be much worse than from outdoor air pollution. This is particularly apparent when a deadly gas is released.

While finite element (FEM) and finite volume methods (FVM) have been developed to a mature stage such that they are now utilized routinely to model complex multi-physics problems, they both require significant effort in mesh generation. Meshless methods are a relative newcomer to the field of computational methods; the term "meshless method" refers to the class of numerical techniques that rely on either global or localized interpolation on non-ordered spatial point distributions. There has been much interest in the development of these techniques since they have the potential of reducing the effort required in model preparation. The meshless method approach finds its origin in classical spectral or pseudo-spectral methods that are based on global orthogonal functions such as Legendre or Chebyshev polynomials requiring a regular nodal point distribution. However, meshless methods use a nodal or point distribution that does not need to be uniform or regular.

3. Objective

Meshless methods are uniquely simple and provide solution accuracies that rival those of finite elements and boundary elements, only without requiring the use of mesh connectivity. What makes these methods attractive is the ease in programming: there is no need for domain or surface discretization, no numerical integration, and there are similar formulations for 2D and 3D models. Several types of meshless methods exist, such as kernel methods, the moving least-square method, partition of unity methods, and radial basis functions. The meshless method use in this research is based on radial basis functions (RBFs) and Kansa's approach [7].

4. Application of Radial Basis Functions

Consider the general, 2-D differential equation

$$Lu = f(x,y) \quad \text{in} \quad \Omega \subseteq R^d, \quad Bu = g(x,y) \quad \text{on} \quad \partial\Omega \tag{1}$$

where L is an arbitrary differential operator, B is an operator imposed as some form of boundary conditions, e.g., Dirichlet, Neumann, Robin or combined. Let $\{P_i = (x_i,y_i)\}$be N collocation points where $\{(x_i,y_i)\}$ are interior points; and $\{x_i,y_i\}_{N+1}$ are boundary points. In Kansa's method, it is assumed that the approximate solution for Eq. (1) can be expressed as

$$u(x,y) = \sum_{j=1}^{N} u_j \phi_j(x,y) \tag{2}$$

where $\{u_j\}$ are the unknown coefficients to be determined and $\phi_j(x,y) = (\|P - P_j\|)$ is some form of radial basis function. Here $r = \|P - P_j\|$ is the Euclidean norm between points $P = (x,y)$ and $P_j = (x_j,y_j)$. The most popular radial basis function is the multiquadric, $\phi(r) = (r^2 + c^2)^{1/2}$, where c is the shape parameter. Substituting (2) into (1), an N x N linear algebraic system can be obtained

$$\sum_{j=1}^{N} (L\phi_j)(x_i,y_i) u_j = f(x_i,y_i), \quad i = 1,2,..N_I \tag{3}$$

$$\sum_{j=1}^{N} (B\phi_j)(x_i,y_i) u_j = g(x_i,y_i), \quad i = N_I+1, N_I+2, ..., N \tag{4}$$

for solving the unknowns $[u_1, u_2, \ldots, u_N]^T$, where N denotes the total number of nodes and N_I the number of internal nodes. The shape parameter, c, is predefined based upon the problem description.

The attractive feature of the localized RBF collocation framework is that it allows field variable derivatives of any order to be estimated by simple inner products of vectors that can be pre-built and stored. In addition, the memory demands of this approach are minimal, as no global collocation

matrix is allocated; only small vectors are stored for every one of the data centers.

Application to Indoor Contamination

Figure 1 (a) shows the configuration of a two-room office complex. Different locations of contaminant sources are denoted by the red dots. Particles are released from a pollutant source in the outer office. The meshless nodal configuration is shown in Fig. 1 (b). If the contaminant is lethal or toxic, then it is critically important for the inhabitants to take evasive action to minimize exposure.

(a) Two-room office (b) Meshless nodal pattern

Figure 1. Office complex layout

Figure 2 shows the concentration (denoted as particle paths) within the two rooms. The pollutant is transported and diffused by the ventilation pattern in the office complex. Source location is particularly important because the pollutant can travel to either side of the desk within the inner office. When first responders arrive at an incident location, it is important that they be aware of the trajectory of the spreading contaminant. The person in the inner office could move to the upper left corner of the room in Fig. 2b or the lower right corner in Fig. 2c until reached by a rescue team.

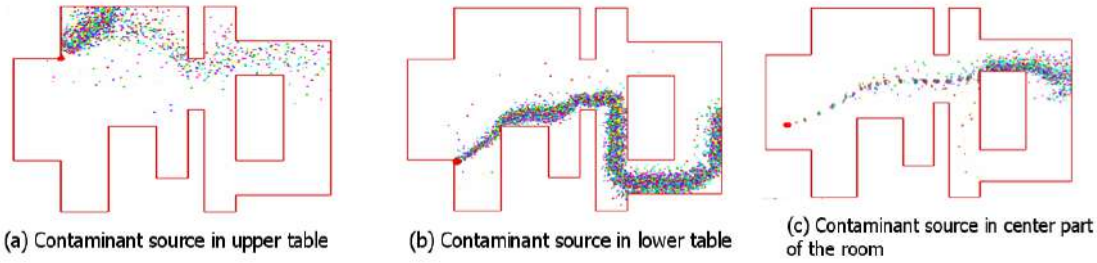

Figure 2. Indoor particle dispersion: (a) upper table, (b) lower table, and (c) door opened.

Application to Mobile Devices

The local meshless technique is used to display 3-D wind fields within the Las Vegas Valley [8]. The model is designed to obtain real-time data from local weather stations and fire departments within the Clark County region of Nevada, which includes the Cities of Las Vegas, North Las Vegas, and Henderson. Wind speeds, directions, and temperatures at each fire department, including access to local National Weather Service data and forecasts, can be used to provide data to the model. Utilizing a connection to the internet, first responders can use their mobile devices, such as phones, tablets, and laptops, to access real-time estimates of the 3-D wind fields. Such models are usually developed through programming packages such as MATLAB, C/C++, FORTRAN, or JAVA. Programming for mobile devices typically requires scripting languages such as Python, Go, Swift (for Apple) or Corona (for Androids). Figure 3 shows output displayed on an Android phone, providing instant wind speed and direction anywhere within the Las Vegas Valley.

Figure 3. Wind Display on Android Phone.

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Vehicle - Bridge Interaction Dynamics and Applications

by Y. B. Yang, Member EUAS

Short Biography

Dr. Yeong-Bin Yang received his Ph.D. degree from Cornell University in 1984. He is a member of Chinese Academy of Engineering (2009) and foreign member of Austrian Academy of Sciences (2007). Currently, he is Honorary Dean of Civil Engineering, Chongqing University, and Professor Emeritus of National Taiwan University (NTU). Also, he is fellow of American Society of Civil Engineers (ASCE) and International Association of Computation Mechanics (IACM), and Editor-in-Chief of International Journal of Structural Stability and Dynamics (IJSSD). In addition, he is President of Asian-Pacific Association of Computational Mechanics (APACM) and Chairman of International Steering Committee of East Asia-Pacific Conference on Structural Engineering and Construction (EASEC).

Previously, he was President of National Yunlin University of Science and Technology (YunTech), Dean of College of Engineering, NTU, Chairman of Department of Civil Engineering, NTU, and President of four societies in Taiwan: Institute of Engineering Education Taiwan (IEET), Chinese Institute of Civil and Hydraulic Engineering (CICHE), Society of Theoretical and Applied Mechanics (STAM), and Chinese Society of Structural Engineering (CSSE). As of now (2018), he has published over 220 referred journal papers, focused on the following areas: structural nonlinear theory and analysis, vehicle-bridge interaction dynamics, and train-induced wave propagation. In each area he has published a monograph.

The vehicle-bridge interaction (VBI) refers to the dynamic interaction between two subsystems, i.e., the moving vehicles and sustaining bridge, mainly in the vertical direction, due to the excitation of the vehicle's movement in the horizontal direction (Yang and Yau 1997). Unlike early researches on the moving load problems, which were focused exclusively on the vibration of bridges, the term VBI is used specifically to highlight the equal importance of both the moving vehicles and bridge responses. This issue is crucial to the design of high speed railways, which now have an operation speed for trains in the range of 300-350 km/hr. Both subsystems are elastic structures and have certain frequencies of vibrations by themselves, in addition to the frequencies implied by the driving speed and rail (track) surface roughness. The two subsystems interact continuously with each other via the contact forces, which are moving as long as the vehicles move. The VBI problem by itself is a nonlinear, time-dependent problem, which in general should be solved by numerical methods, such as the finite element method. It is only under certain conditions that analytical solutions in closed form can be obtained.

Inspired by his series of research on VBI problems since the 1990s, the vehicle scanning method (VSM) was firstly proposed by the author in 2004 for extracting the vibration frequencies of bridges using a moving test vehicle (Yang et al. 2004). This technique was then extended to the construction of mode shapes of bridges (Yang et al. 2014), and further to the damage detection of bridges (Zhang et al 2018).

In this short article, the author will summarize some of the major contributions carried

out by him and his research group mainly along the lines of VBI and VSM, with potential applications highlighted.

1. Vehicle-bridge interaction element

The first need for studying the VBI problems is to develop an accurate and efficient element for analysis of railway bridges traveled by a train with a number of vehicles (Yang and Yau 1997). The train is modeled as a series of sprung masses and the bridge with track irregularities by beam elements. Two sets of equations of motion are written, each for the bridge and the sprung mass. To resolve the problem of coupling between the two subsystems, the sprung mass equation is first discretized using Newmark's finite difference formulas and then condensed to that of the bridge element in contact. The element derived is referred to as the VBI element, which has the same number of degrees of freedom (DOF) as the parent element, and can be easily implemented in analysis software using the conventional assembly procedure. This element was later enhanced to include the effect of pitching of the moving vehicle (Yang et al. 1999).

2. Impact factor for bridges due to moving loads

Previously, the impact factor induced by moving vehicles was related only to the length or frequency of the bridge in some bridge design codes. This is not physically sound. By modeling a vehicle as sprung masses and a bridge by beam elements, a parametric study is performed for various simple and three-span continuous beams traversed by five-axle trucks (Yang and Lin 1995; Yang et al. 1995). Central to this study is the adoption of a nondimensional speed parameter *S*, defined as the ratio of the vehicle's driving frequency to the first frequency of the beam. Based on the parametric study, it is concluded that the impact factors for the deflections, bending moments, and shear forces at the midpoints of simple beams are linearly proportional to the speed parameter *S*, and that these formulas can be multiplied by certain modification factors to yield formulas for continuous beams and support shears.

3. Optimal design length for railway bridges

To investigate the vibration of simple beams under the passage of high speed trains, a train is modeled as the composition of two subsystems of wheel loads of constant intervals, with one for all the front wheels and the other for the rear wheels. Using the moving load model, the key parameters that govern the dynamic responses of the beams are identified analytically and verified by a numerical analysis. Based on the condition of cancellation for the waves generated by the moving loads, optimal design criteria that are irrelevant of vehicle speed are proposed for suppressing the resonant responses of simple beams. In designing highspeed railway bridges, such criteria can be adopted in selecting the span length of simple beams, given the car length and axle distance of the train model to be used (Yang et al. 1997).

4. Riding comfort of highspeed trains

The vibration of simple and three-span continuous beams traveled by highspeed moving trains is studied in terms of the non-dimensional speed parameter *S*, defined as the ratio of the vehicles' exciting frequency to the first frequency of the beam. It was indicated that the moving load model is generally good for simulating the bridge response, but the sprung

mass model should be used instead for obtaining the vehicles' response. If the characteristic length, rather than the span length, is used for continuous beams, then both the simple and continuous beams will reach their peak responses at the same critical speed *S* under the same wheel loads. Factors such as rail irregularity, ballast stiffness, suspension stiffness and suspension damping can drastically affect the riding comfort of the rail cars moving over simple beams, but their effects are comparatively small for continuous beams (Yau et al. 1999).

5. Derailment for highspeed trains under earthquakes

The dynamic analysis of trains moving over bridges shaken by earthquakes requires not only acceleration, but also velocity and displacement of the ground motion (Yang and Wu 1999). Four earthquakes adopted as the input excitations, including the 1999 Chi-Chi Earthquake, were normalized to have a moderate intensity. The results indicate that a train initially resting on the bridge can stay safely under the ground motions considered, if the bridge and track structures remain elastic during the earthquake. The vertical component of ground motions affects significantly the stability of the train-rail-bridge system. As an initial attempt, safety, possible instability and instability regions were established in a three-phase plot for the train running over the bridge for each of the earthquakes considered, from which the maximum allowable speed for the train to run safely is obtained.

6. Resonance of trains moving over a series of bridges

For a highspeed train with a series of cars moving over a bridge, train-induced resonance on the bridge may occur when any of the bridge frequencies coincides with any of those implied by the wheel loads. On the other hand, for a vehicle moving over a series of identical bridges at constant speeds, bridge-induced resonance on the vehicle may occur when any of the vehicle frequencies coincides with any of those of the bridges. A complete coverage for the train- and bridge-induced resonances on the train-bridge system was presented by Yang and Yau (2017) using both the analytical and numerical means, with focus placed on the mechanism of resonance between the two subsystems of the train and bridges. The numerical results indicate that the train-induced resonance on the bridges takes place at higher speeds, but the bridge-induced resonance on the train cars at lower speeds.

7. Extraction of bridge frequencies from moving vehicles

The idea of using a moving vehicle to detect the frequency of the sustaining bridge was firstly explored by Yang et al. (2004). To identify the key parameters dominating the vehicle-bridge interaction response, while illustrating the key phenomena involved, assumptions that lead to closed-form solutions are adopted in the analytical study. Particularly, a vehicle is modelled as a sprung mass, and a bridge as a simply supported beam considering only the first mode of vibration. The concept of extracting bridge frequencies from a passing vehicle, however, is not restricted by the aforementioned assumptions, as was demonstrated in the independent finite element analysis, which virtually does not rely on any modeling assumptions. The feasibility for extracting the bridge frequencies from the dynamic response of a passing vehicle is confirmed, along with directions for future research identified.

8. Using moving test vehicle to construct mode shapes of bridges

A theoretical algorithm was presented for constructing the mode shapes of a bridge from the dynamic responses of a moving test vehicle over the bridge based mainly on the Hilbert transform (Yang et al. 2014). Unlike the conventional approach that relies on a limited number of sensors deployed on the bridge, the present approach is rich in spatial information, since the moving test vehicle can virtually touch each point of the bridge axis, which enables the mode shapes of the bridge to be constructed with high resolution. The other advantage is that only one or few sensors need to be installed on the test vehicle, but not on the bridge. Factors affecting the accuracy in constructing the bridge mode shapes are studied, such as vehicle speed, random traffic, and road surface roughness. It was verified that the approach is feasible for the test vehicle moving at constant and low speeds.

9. Damage detection of bridges by moving test vehicle

To further the technique of vehicle scanning method for bridges, the contact-point response of a moving test vehicle is adopted for the damage detection of bridges (Zhang et al. 2018). First, the contact-point response of the vehicle moving over the bridge is derived both analytically and in central difference form (for field use). Then, the instantaneous amplitude squared (IAS) of the driving component of the contact-point response is calculated by the Hilbert transform, making use of its narrow-band feature. The IAS peaks serve as the key parameter for damage detection. In the numerical simulation, a damage (crack) is modeled by a hinge-spring unit. The feasibility of the proposed method to detect the location and severity of a damage or multi damages of the bridge is verified. Also, the effects of surface roughness, vehicle speed, measurement noise and random traffic are studied. In the presence of ongoing traffic, the damages of the bridge are identified from the repeated or invariant IAS peaks generated for different traffic flows by the same test vehicle over the bridge.

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Systems Analysis of Multiple Steady Behavior in Glucose Metabolism

by Wei-Shou Hu, Member EUAS

Short Biography

Wei-Shou Hu received a B.S. from National Taiwan University in Agricultural Chemistry, a S.M and a Ph.D. in Biochemical Engineering from Massachusetts Institute of Technology. He joined the Department of Chemical Engineering and Materials Science at the University of Minnesota upon receiving his Ph.D. where he is now a Distinguished McKnight University Professor. He started his career working on cell culture bioprocessing at a pivotal point of biotechnology, as mammalian cell culture became the major vehicle for the production of recombinant proteins. These protein therapeutics are now keys to the treatment of many major diseases. He initiated the Engineering Foundation Conference on Cell Culture Engineering twenty-eight years ago that is still one of the most important forums for the bioprocess technology and has had a great impact on the biotech industry. The short course, Cellular Bioprocess Engineering, that he initiated thirty years ago has trained thousands of biotechnologists in this area and is still thriving.

Current research efforts emphasize exploiting genomics and proteomics in advancing bioprocess technology, and applying systems analysis to generate new understanding of metabolic and gene expression regulation. He leads a Systems Biotechnology for Chinese hamster ovary cells (CHO) consortium consisted of pharmaceutical companies to drive genomic and systems research for bioprocess technology. He co-authored the textbook Bioseparations and co-edited the monograph Cell Culture Technology for Pharmaceutical and Cell-Based Therapies. His educational effort includes a widely known training course on cell technology. Over the past quarter century this annual course has been offered in five continents and helped trained thousands of scientists and engineers for pharmaceutical and biotech industry around the world. Prof. Hu also authored Cell Culture Bioprocess Engineering as a culmination of his long-standing cell technology research. His recent new textbook Engineering Principles in Biotechnology is another hallmark of his contribution to biochemical engineering.

For his contribution to cell culture engineering he received the inaugural Merck Award on cell culture engineering and the Lifetime Achievement award from the Society of In Vitro Biology. He was also recognized for his contribution in biochemical engineering by the Marvin Johnson Award from the Biochemical Technology Division of the American Chemical Society, the distinguished service award of Society of Biological Engineers, a special award from Asia Pacific Biochemical Engineering Conference, the Amgen Award for Biochemical Engineering, as well as both the distinguished service award and the Division award from Division of Food, Pharmaceuticals and Bioengineering of the American Institute of Chemical Engineers.

Glycolysis is the conduit of glucose metabolism for energy generation. It also supplies precursors for biosynthesis of cellular materials. The flux of glucose into glycolysis is high in cancer cells as compared to normal adult tissues. A vast amount of the glucose consumed is diverted towards lactate production; a phenomenon known as the Warburg

effect. This behavior of fast glucose consumption is also typical of highly proliferative cells such as epithelium cells and cells cultured *in vitro*. In resting tissues, the glucose flux is low and much less lactate is produced from glucose metabolism. Why such differences in glycolysis activity across cell types is still a subject of debate. The variation in glycolysis flux is the results of transcriptional as well as allosteric feed-back and feed-forward regulations exerted by the intermediate metabolites on its enzymes. A number of enzymes play pivotal roles in controlling glycolysis flux, including phosphofructokinase (PFK), pyruvate kinase (PK) and phosphofructokinase /fructose-2,6-bisphosphatase (PFKFB)). Each of these enzymes have multiple isoforms which have different kinetic behavior and are subjected to contrasting allosteric regulations. The make-up of isoforms and the expression levels of glycolysis enzymes dictate the kinetic behavior of the pathway.

An additional mechanism of flux regulation in glycolysis is through signaling pathways. Protein kinases A/B/C (PKA, PKB and PKC) affects the glycolysis flux through the modulation of PFKFB activity. Since their activity is linked to cell's growth rate regulation, they provide the link between growth rate regulation and glycolysis flux.

The composition of isozymes in glycolysis, through multiple layers of regulation, is thus pivotal to the flux control and plays a key role in growth control and physiological balance. Over the last four decades, the kinetic behavior of isoforms of individual glycolytic enzymes has been examined in detail. We have taken a systems biology approach to study the flux states of glycolysis pathway. Using a mathematical model that employs mechanistic rate equations for enzyme kinetics and the transcript levels as the first approximation of the level of enzymes, we demonstrate that glycolysis exhibits a classical multiple steady state behavior in terms of its flux with respect to the glucose concentration and lactate concentration. The multiplicity of steady states separates cell metabolism into distinct states: high glycolytic flux states and low glycolytic flux states (Figure 1).

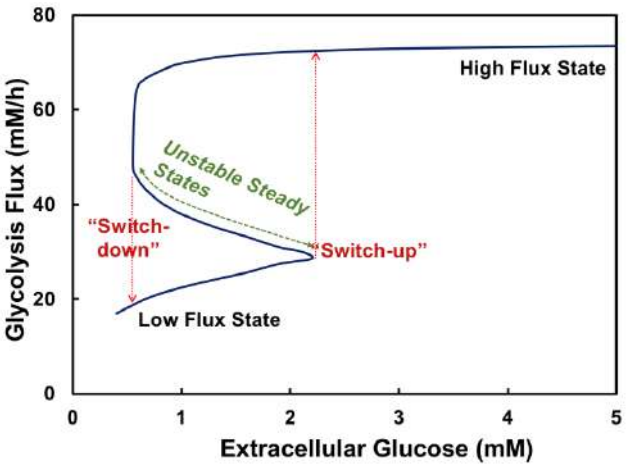

Figure 1. Multiplicity of steady states in glycolytic activity.

The revelation of the multiple steady state behavior in glycolytic flux not only provides new insights on the regulation of cell metabolism, but also shed light on some metabolic enigma in cell culture bioprocessing. Mammalian cells are the predominant host cells for the production of therapeutic recombinant proteins. In the past three decades, fed-batch culture, wherein feed containing nutrients are regularly added to the culture to replenish those consumed to sustain longer cell growth and production period, has become the prevailing form of process. Over a period of about two weeks, concentrated medium is fed extensively to reach a high cell concentration. Concurrently the product, as well as the

metabolites, especially lactate, accumulate to high levels. The concentration of glucose and the level of lactate accumulated in culture greatly exceed the physiological level.

Cells in the late stages of a fed-batch culture sometimes switch their metabolism from lactate production to lactate consumption even in identical culture conditions. This behavior is unpredictable and has been shown to have a drastic effect on productivity. The cultures that switch from a high glucose flux state to a low flux state have a high productivity, while those which continue to produce high levels of lactate have lower productivity. As nucleotide sugar precursors for glycan synthesis are supplied from glucose metabolism, the variations in glucose metabolism also affects the glycan pattern of therapeutic proteins. Thus, the often-seen unpredictability of metabolic switch to lactate consumption is problematic, and a better control of the cell metabolism is important to the product yield and quality.

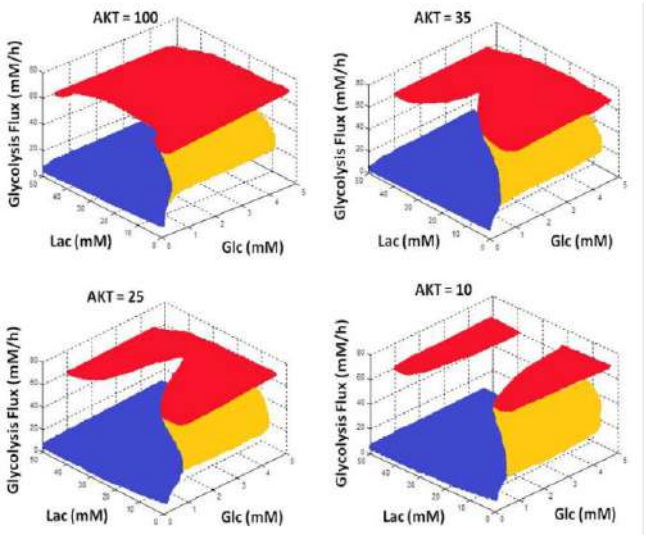

Figure 2. Effect of glucose and lactate on glycolytic flux at different AKT activities: 100%, 35%, 25% and 10%. The red and blue surfaces are stable steady states representing the high and low glycolytic flux states, respectively. Yellow surfaces are unstable steady states representing the intermediate glycolytic flux states.

The topology of the bistable region is greatly influenced by lactate concentration (Figure 2, AKT=100). At the high levels of typical fed-batch culture, the inhibitory effect of lactate on PFK becomes very pronounced.

The topology is affected by growth rate via AKT signaling (Figure 2). AKT plays a key role in multiple cellular processes including cell proliferation and glucose metabolism. A decrease in the growth rate is accompanied by the decrease in the phosphorylated AKT (pAKT) levels, which in turn affects the kinase activity of the bifunctional enzyme PFKFB. At a slower growth rate, the shift down (from a high flux state to a low flux state) glucose concentration increases, making it easier to switch to the low flux state. At even lower growth rate, a valley opens up. The peculiar topology happens at the high levels of glucose and lactate seen in fed-batch processes but not encountered under physiological concentrations.

This model was used to explain the frequently seen “unpredictable” behavior of metabolic shift in bio-manufacturing. During the exponential growth phase, the metabolism is at a high flux state. In fed-batch culture, glucose is added to the medium periodically. As the growth rate slows down and the topology of the steady state changes, the metabolic state may drift to the valley and switch to a low flux state (Figure 3, trajectory A-B-C-D-E). Depending on the topology of the steady states, feeding of glucose may cause the trajectory to move away from the valley and the metabolism is then trapped in a high flux state (trajectory B-F-G in Figure 3).

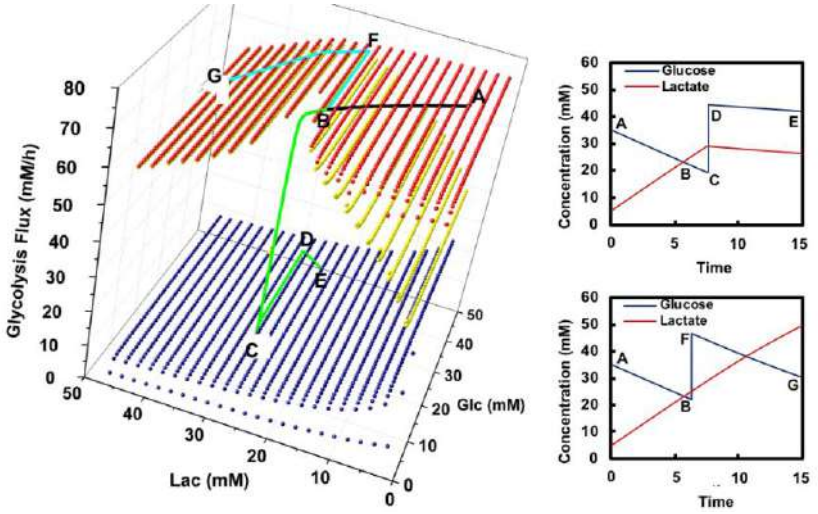

Figure 3. Transient simulations of cultures with and without metabolic shift. Cells at exponential stage are initially cultured in high glucose and low lactate concentrations and exhibit high growth rate/AKT activity. (A-B) As the culture progresses, AKT activity decreases (pAKT = 0.17), glucose is consumed and lactate accumulates in the culture such that the trajectory follows the curve A-B in the top plane, then falls from B to C at a low flux state. The addition glucose (C to D) will not change the low flux state. In a different scenario (B-F-G), with an early glucose feeding, no metabolic shift is possible.

The model was extended to multi-scale integrating the intracellular metabolism with the macroscopic cell growth in a continuous bioreactor. Through model simulations, we show that multiplicity of steady states is present in a range of dilution rates in continuous culture and demonstrate the trajectory that one can employ to guide the culture to the desired steady state.

Recently the model was further extended to consider the effect of AMPK signaling pathway on glycolysis. The results addressed another prominent issue of switching from a low glycolytic flux state to a high flux state and provided again insight into another "unpredictable" behavior of cells under bioprocess culture conditions. The model is currently being applied in mathematical optimization to identify genetic manipulation that will fulfill certain objective functions aiming to alter cell metabolism under different growth conditions.

Fire Risk Assessment & Safety Design of Buildings & Urban Areas

by Jinhua Sun, Member EUAS

Short Biography

Education and Positions

2004~ Vice Director of State Key Laboratory of Fire Science of China
2002~ Professor, University of Science & Technology of China
1999~2002 Research Professor, Japan Science and Technology Agency, Japan
1996~1999 Ph.D., The University of Tokyo, JAPAN
1988~1996 Associate Professor, Anhui University of Science & Technology, China
1986~1988 M. Sc., Nanjing University of Science and Technology, China
1983~1986 Assistant Professor, Anhui University of Science & Technology, China
1979~1983 B. Sc., Nanjing University of Science and Technology, China

Professional Activities

Vice-chairman of Asia-Oceania Association for Fire Science and Technology (2007~)
Committee Member of the International Association for Fire Safety Science(2008~2017)
Committee Member of the National Science and Technology Award (2010~)
Academic Committee Member of University of Science and Technology of China (2009~)
Safety expert committee Anhui Province, Civil blasting group leader(2009~)
Member of Science and Technology Award Committee, Ministry of Public Security (2007~)
Member of Academic Committee of urban safety and disaster prevention, Urban Planning Society of China (2005~2015)
Evaluation expert in international scientific and technological cooperation program, Ministry of Science and Technology of China (2005~)
Executive director of Anhui Fire Protection Association (2005~)
Associate Editorial or Editorial Board of five International Journals(2010~)
Editorial Board of nine national Journals(2003~)
Academic Committee Member of China Fire Protection Association(2003~)

Honors and Awards

National Science and Technology Progress Award, First-class Award, China (1993)
Member of Hundred Talent Program, Chinese Academy of Sciences (2001)
Outstanding Member Hundred Talent Program, Chinese Academy of Sciences (2005)
National Science and Technology Progress Award, Second-class Award, China (2006)
Science and Technology Award for Young Scientist, Anhui Province (2006)
Safety Science and Technology Award of State Administration of Work Safety, Second-class Award (2006)
Beijing Science and Technology Award, Third-class Award, Beijing (2008)
Teaching Award of Anhui Province, First-class Award, Anhui Province (2010)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2014)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2014)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2017)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2017)
Science and Technology Innovation Award, First-class Award, China Fire Protection Association (2018)

Fire is a kind of disaster that occurs at a high frequency and can be extremely harmful to human lives and properties. Professor Sun Jinhua has long been devoted to academic research and education in the area of fire science and fire protection. He has made substantial accomplishments in a number of fields in fire safety science and engineering, including fire risk assessment, performance-based fire protection design, building fire safety, industrial fire safety, fire safety in new energies. He led as a PI more than 20 important national research projects, such as the National "973 Program", key projects funded by National Natural Science Foundation of China (NSFC), the "11th Five-Year plan" and the "13th Five-Year Plan" national key R&D program, the sixth Framework Project of the EU International Cooperation Program in Science and Technology, NSFC general projects, and "Outstanding Talents" project funded by the Chinese Academy of Sciences. He has published more than 300 journal papers, more than 100 conference papers, and 11 academic books or book chapters.

Major Research Areas

1. Methods for fire risk assessment and safety design of buildings and urban areas

Buildings and urban areas are the most basic and important places for human life and production activities. Building and urban fires that occurs frequently are a serious threat to human life and property. It is an imperative demand in the development of human society and economy to evaluate fire risk in buildings and urban areas, develop effective scientific methods for fire safety design, and optimize the allocation of urban fire-fighting resources. The final goal is to achieve reliable and economic prevention and control of building and urban fires.

1) **Fire risk assessment and performance-based fire protection design for buildings**. Although the occurrence and development of fires are stochastic processes in nature, fire process follows its own laws and can be predictable when the initial and boundary conditions of its development are determined. Starting from the smallest urban unit, i.e. a single building, we develop a methodology of building fire risk assessment that couples statistical theory and fire dynamics. Quantitative risk assessment of building fires can be realized through this method. We then developed a method of building fire protection based on fire risk assessment.
2) **Urban area fire risk assessment and fire protection capacity optimization design.** As the economy grows rapidly in China, cities becomes larger and larger. Meanwhile, a large number of commercial centers and industrial parks emerge. Traditional safety design methods for urban areas becomes obsolete nowadays under the new economic and social situations. We extended the idea of building fire risk assessment and safety design to urban areas, and developed evaluation methods of fire risk and fire protection capability for urban areas. In addition, we proposed optimized allocation and scheduling methods of fire station, fire protection capacity, and emergency resources based on regional fire risk assessment. Overall, the accomplishments in theories and methods of fire risk assessment and safety design for buildings and urban areas have provided scientific and technical supports and guidance for the fire risk assessment and performance-based fire protection design of hundreds of major construction projects in China, as well as planning of fire safety, distribution of fire stations and allocation of fire protection facilities in some domestic cities.

2. Theory of fire dynamics and methods of fire prevention and control for high-rise buildings

With the rapid development of economy and society, the fire phenomena and dynamics high-rise buildings are quite different from that of conventional buildings because of the complexity and diversity of building functions and the extensive use of new materials such as insulation materials on exterior walls. The fire safety situation of high-rise buildings is very serious all over the world, especially in China. Fire prevention and control in high-rise buildings is a worldwide tough problem. Focusing on the fire safety of high-rise building in China, we proposed a theory that includes three lines of defense of safety, i.e., the intrinsic safety, process safety and target safety. This theory helps ensure fire safety in high-rise buildings.

1) **Safety design and preparation of thermal insulation materials of building.** Starting from the intrinsic safety of materials, we developed and improved a multi-scale experimental method for analyzing fire characteristics and a fire risk assessment method of thermal insulation materials and thermal insulation systems. In addition, based on the flame retarding methods with synergistic effects of condensed and gas phases as well as the methods of smoke suppression and attenuation using nanocomposite catalytic, we developed a fire safety design method of organic insulation materials for exterior walls and prepared a safe exterior wall insulation material.
2) **Prevention of three-dimensional internal-external interactive fire spread of high-rise buildings.** Aiming at revealing the dynamics of fire and smoke spread of high-rise buildings, we proposed for the first time a theory of three-dimensional internal-external interactive fire spread of high-rise buildings. We also developed a prevention method of three-dimensional fire spread. Furthermore, we revealed the mechanisms and laws underlying the fire smoke transport under multiple forces in high-rise buildings. We finally developed numerical prediction methods of smoke transport and control methods of smoke in high-rise buildings.

3. Theories and methods of fire prevention for new energies

Great interest in developing and utilizing new energy sources is generated all over the world. In particular, developing vehicles driven by new energies is currently a booming field of research. However, safety issues in production, storage, transportation, and use of new energies becomes more and more prominent, especially for the vehicles powered by lithium-ion batteries. The frequency of fire and explosion accidents is extremely high for electric vehicles. This seriously restricts the development of the new energy industry. Aiming at solving the safety problems of lithium-ion batteries, we first carried out a series of studies on the characteristics and mechanisms of fire and explosion. Then we developed methods and techniques for preventing and controlling fires and explosions of li-ion batteries. In addition, we have conducted fundamental research of safety of hydrogen as a new energy carrier.

1) **Fire and explosion characteristics of lithium-ion batteries and the corresponding prevention and control methods.** In our research, the intrinsic relationships of fire characteristics and heat release rate of lithium-ion batteries with state of charge were obtained. The underlying mechanisms of fire and explosion of lithium-ion batteries were revealed in detail. Intrinsically safe electrolytes that can prevent decomposition and combustion of lithium-ion batteries were developed. This effectively improves the

safety of lithium-ion batteries. Based on the fire and explosion characteristics of battery materials, the thermal runaway process of battery, and the heat generation characteristics in charge and discharge cycles, a three-level warning technique for ensuring safe operation of large-scale lithium-ion energy storage systems is proposed. A method of fire protection design was proposed. This design can decrease the temperature of battery by cooling and equip battery with a fire extinguishing function that can be used for a number of times. These methods and techniques developed effectively solves parts of the technical problems of fire protection for the lithium battery systems.

2) Hydrogen Fire and explosion safety. The generation, propagation and enhancement (or attenuation) of shock waves during high-pressure hydrogen leak or release, and the influences of key parameters such as initial pressure, gas temperature and pipe structure/size on the spontaneous ignition of high-pressure hydrogen leak were investigated systematically. An in-depth study of the dynamics process of the growth of flame kernel produced by spontaneous ignition of high-pressure hydrogen was conducted. The critical conditions and parameter range of flame kernel growth were given. The mechanism of subsequent flame propagation was also scrutinized. A new phenomenon of premixed hydrogen/air flame dynamics was discovered, i.e., the distorted tulip flame. The formation mechanism of this new phenomenon was elucidated and a theoretical model was developed.

Innovations in Radiation Materials Science

by Gary Was, Member EUAS

Short Biography

Professor Was received his ScD from MIT in 1980. He is the Walter J. Weber, Jr. Professor of Sustainable Energy, Environmental and Earth Systems Engineering, and holds appointments in Nuclear Engineering and Radiological Sciences, and Materials Science and Engineering at the University of Michigan. He has held positions as Director of the Michigan Memorial Phoenix Energy Institute, Associate Dean of the College of Engineering and Chair of the Nuclear Engineering and Radiological Sciences Department. Professor Was' research is focused on materials for advanced nuclear energy systems and radiation materials science, including environmental effects on materials, radiation effects, ion beam surface modification of materials and nuclear fuels. Most recently his group has led the development of proton irradiation as a technique for emulating neutron irradiation effects in reactor structural materials and has conducted some of the first stress corrosion cracking experiments of austenitic and ferritic alloys in supercritical water.

During his tenure at the University of Michigan, Professor Was has graduated 39 Ph.D. students, created several graduate level courses dealing primarily with irradiation effects on materials, ion beam modification of materials and nuclear fuels. He served as chair of the Nuclear Engineering Department Heads Organization and co-authored the first ASEE report on Manpower in the Nuclear Industry. He has helped to organize more than a dozen technical symposia and is a member of the American Society for Engineering Education, Materials Research Society, ASM International, The Minerals, Metals and Materials Society, the NACE International, Sigma Xi and Tau Beta Pi. He is director of three major laboratories at the University of Michigan: the Michigan Ion Beam Laboratory for Surface Modification and Analysis, the High Temperature Corrosion Laboratory, and the Irradiated Materials Testing Laboratory. Professor Was received the Presidential Young Investigator award from NSF in 1985 and in 1994 he received the Excellence in Research Award from the College of Engineering. He was awarded the Champion H. Matthews Award from TMS, the Outstanding Achievement Award and Special Achievement Award by the Materials Science and Technology Division of the American Nuclear Society, the 2008 Henry Marion Howe Medal from ASM, the Lee Hsun Award from the Chinese Academy of Sciences, the Mishima Award from ANS and the Glenn Murphy Award from ASEE. He is a Fellow of The Minerals, Materials and Metals Society (TMS), the Materials Research Society, ASM International, NACE International and the American Nuclear Society. Professor Was has published over 270 technical articles in referred, archival journals, presented over 480 conference papers, and delivered over 230 invited talks and seminars, published a graduate level textbook on

Radiation Materials Science in 2007 and a second edition in 2017. He serves as Editor-in-Chief of the Journal of Nuclear Materials.

High Fidelity Simulation of High Dose Neutron Irradiation with Ions

The promise for developing new, advanced nuclear reactor concepts that significantly improve on the safety, economics, waste generation and non-proliferation security of commercial nuclear power reactors, and the extension of life of existing light water nuclear reactors rests heavily on understanding how radiation degrades materials that serve as the structural components in reactor cores. In high dose fission reactor concepts such as the sodium fast reactor (SFR), lead fast reactor (LFR), molten salt reactor (MSR) and the traveling wave reactor (TWR), structural materials must survive up to 200 displacements per atom (dpa) of damage at temperatures in excess of 400°C. Traditionally, research to understand radiation-induced changes in materials is conducted via radiation effects experiments in test reactors, followed by a comprehensive post-irradiation characterization plan. Today, there are a diminishing number of test reactors – both thermal spectrum and fast spectrum – in which to conduct such irradiations. Irradiations require long irradiation periods followed by the very slow process of handling irradiated materials, all of which results in extremely high costs.

A promising solution to the problem is to use *ion* irradiation that can produce high damage rates with little or no residual radioactivity. The advantages of ion irradiation are many. Dose rates are factors of 10^2 to 10^4 times higher than in test reactors, which means that 200 dpa can be reached in days or weeks instead of decades. Because there is little activation the samples are not radioactive. Control of ion irradiation experiments is much better than experiments in reactor. The high rate at which ion irradiations can be conducted, coupled with the absence of residual radioactivity are the key attributes that make this route to advancing our understanding of radiation effects so attractive. One of my major projects is the development of the capability to predict the evolution of microstructure and properties of structural materials in-reactor and at high doses, using ion irradiation as a surrogate for reactor irradiations. Such a project requires comparison with reactor irradiations and so our project involves not only ion irradiations, but reactor irradiations to high dose, followed by microstructure characterization of both, along with assessment of mechanical properties of the irradiated materials.

To date, ferritic-martensitic alloys T91 and HT9 and austenitic alloy 800H have undergone irradiations in reactor and with ions to damage levels up to 50 dpa. Agreement between the microstructures of ion and neutron irradiated samples is generally excellent. Microstructure models are being developed to provide predictive capability and the first results of micro- and nano-mechanical property comparison are encouraging. The overall goal is to establish a physics-based methodology for conducting ion irradiations in a way that replicates the key aspects of the microstructure of alloys irradiated in reactor. This will provide the capability for ion irradiation to act as a surrogate for reactor irradiations for a large fraction of radiation effects projects and may also lead to acceptance by regulators to allow ion irradiation data to be used in component design and safety certification.

Irradiation Assisted Stress Corrosion Cracking

The combination of radiation damage and an aggressive environment is a primary life-limiting process for structural components in nuclear reactor cores. Intergranular stress corrosion cracking in irradiated materials is one of the most important and yet poorly understood phenomena that limits the lifetime of metal alloys in these aggressive, high temperature environments. Much has been studied on the role of the environment and alloy composition, but relatively little attention has been paid to deformation mode. In fact, in many high strength alloys, deformation is heterogeneous rather than homogeneous, and is a potential cause of IG cracking. In particular, strain localization can be a controlling phenomenon in irradiated materials under extreme conditions. The key to the IG cracking mechanism likely resides in the nature of the interaction between localized deformation bands and the grain boundaries. Unfortunately, the interaction between localized deformation and grain boundaries is a problem that needs to be understood at the atomic scale and is very difficult to study both experimentally and computationally. In recent years new experimental, theoretical, and computational techniques have become available to study properties at length and time scales not accessible previously. Experimental techniques are able to deal with smaller and smaller length scales whereas simulation techniques using massively parallel processing can deal with an increasing number of atoms and for the first time, the two approaches are merging. This convergence of simulation and experiment can significantly contribute to the development of new, engineered materials that tolerate irradiation under extreme conditions. This proposal describes such a program for understanding intergranular cracking in reactor materials.

Using novel experimental techniques employing in-situ capability, pre-determined and pre-characterized geometries for dislocation channel - grain boundary interaction, and molecular statics and molecular dynamics modeling of channel - boundary interaction, my group looking at the processes by which IG cracking initiates in irradiated austenitic Fe-Cr-Ni alloys in aggressive media at high temperature. we have determined the local conditions for initiation of IASCC. These are the development of a high normal stress localized at the intersection of the dislocation channel and the grain boundary, driven by the intense dislocation activity in the channels. We have also determined that it is the discontinuous dislocation channels, ones that terminate at the grain boundary, that are primarily responsible for the observed IG cracking in high temperature water. It is at these locations where stresses are the highest, and we have further established high resolution electron backscattering diffraction (HREBSD) as a viable method for quantifying the strain and stress tensors at these locations. By virtue of the strong bond between the oxide and the underlying metal alloy, the high stresses are relieved only by the rupture of the oxide film above the grain boundary, allowing contact between the high temperature water environment and the freshly exposed metal. In this regard, the corrosion mechanism responsible for the intergranular cracking remains to be established. We have begun exploring local compositional variations of the oxide on the surface, the grain boundary, and within cracks especially the crack tip. In this effort we seek to link the rupture of the oxide film to a critical local stress with structural and compositional changes in the grain boundary driven by the corrosion event.

A key feature of the approach has been the implementation of a mesoscale science approach that provides linkage from atomistic simulations of dislocation responses to the accommodation and emission of dislocations from grain boundaries, through direct

observation of dislocations with irradiation defects and grain boundaries, to macroscale experiments. The consequence of this combined effort has been the identification of the factors most likely responsible for establishing not only the local stress state at grain boundaries prone to failure but also their location with respect to the macroscopic applied stress. That is, the grain boundaries and local conditions at which disruption of the surface oxide and hence, exposure to the water environment is most probable, have been identified. Having isolated these conditions, the team is poised to address why cracking does not occur at every grain boundary that is favorably oriented, why it remains isolated at one channel over others along the same grain boundary, and why the environment-metal interaction is key to cracking. With these questions in mind, the overall objective is to determine the basic processes by which localized deformation in irradiated materials leads to intergranular cracking in alloys in aggressive environments at high temperature.

Stimuli-responsive Polymers: Shape Memory, Damage Healing and Actuation

by Guoqiang Li, Member EUAS

Short Biography

Professor Guoqiang Li is currently LSU Alumni Professor and John W. Rhea, Jr. Professor of Mechanical Engineering at Louisiana State University (LSU). He is also serving as Associate Vice President in the Office of Strategic Initiatives at LSU. Li received his B.S. degree from Hebei University of Technology in 1985, M.S degree from Beijing University of Technology in 1988, and Ph.D. degree from Southeast University in 1997, all in Civil Engineering with his focus on polymer modified asphalt and cement based composites. In 1997, Li joined LSU Mechanical Engineering as a postdoctoral research associate, with his focus on polymer composite materials and structures. He was promoted to Research Assistant Professor in 2000. In 2003, Li was hired as a tenure-track Assistant Professor at both LSU and Southern University (joint faculty appointment). In 2007 and 2008, he received his early promotion to Associate Professor with tenure at Southern University and LSU, respectively. Li was promoted to Professor in 2012, at both institutions, all considered to count as early promotions. He was then appointed as Associate Vice President in the Office of Strategic Initiatives at LSU in 2013.

A signature of Li's research career to date is that he has acquired strong multidisciplinary knowledge and skills bridging Science and Engineering, particularly composite materials and solid mechanics and their applications in engineering structures. Because of his multidisciplinary knowledge and ground-breaking ideas, Li has been able to secure an impressive level of funding with 58 research grants from federal and state funding agencies and industry, including NSF, NASA, DoE, DoD, FHWA, TRB, ARO, AFRL, USACE, USDA, etc., with a total research funding of over $40 million.

Li is a disciplined scholar, and his ability to identify and independently develop new research areas is demonstrated by his widely disseminated research through scholarly publications. So far, he has published 200 refereed journal papers, including some flagship journals in solid mechanics such as Journal of the Mechanics and Physics of Solids, in polymer science such as Progress in Polymer Science, in basic science such as Nature Communications, and in engineering such as ASCE Journal of Transportation Engineering. In addition, he published the first book on shape memory polymer based self-healing structures by John Wiley&Sons in 2014 and co-authored a book on adhesively bonded composite joint in 2009. Furthermore, Li published 12 book chapters and edited 1 book published by Elsevier. In addition, he published over 150 conference proceedings/presentations in professional conferences and delivered over 70 invited talks and seminars. His research accomplishments have been well recognized. Sixteen journal papers have been among the most cited papers since 2010, based on either Google Scholar and/or SCOPUS, and three papers are among the 1% Highly Cited Papers per ISI Web of Science.

Li is one of the pioneers of using micromechanics to conduct stress analysis and predict

modulus and tensile strength of cement concrete and asphalt concrete, and using the results to guide development of cement-asphalt emulsion composites, recycling of asphalt pavement, and recycling of waste tires in concrete. He developed advanced grid stiffened composite tubes to confine concrete and achieved remarkable enhancement in compressive yield strength and ultimate strength. Further, he enhanced the fire tolerance of such composite structures by using nanoclay based composite. Later, his group developed cohesive law models to predict the Mode I, Mode II, and mixed Mode I&II fracture in adhesively bonded joints, and found ways to experimentally obtain the cohesive law through a combination of local and global tests, including the effect of adhesive thickness on the cohesive law, energy release rate, and fracture toughness. Li proposed the bioinspired close-then-heal (CTH) strategy for healing wide-opened macroscopic cracks by mimicking the self-healing of human skin. This scheme first closes cracks through constrained shape recovery, either constrained expansion of compression programmed shape memory polymer (SMP) matrix, or constrained shrinkage of embedded, tension programmed SMP fibers or twisted-then-coiled polymeric artificial muscles; and then heals the narrowed cracks intrinsically or extrinsically. This strategy has been widely regarded in the literature as the most practical approach to heal macroscopic cracks such as those induced by impact loading. As a result, this strategy has received three patents. Li also published the first book in this area of study. For chemically cross-linked amorphous SMPs, a grand challenge is the low energy storage capability and low recovery stress in rubbery state, significantly limiting their applications. Li discovered a new strategy of using enthalpy to store energy through chemical bond length increase, in addition to the well-known entropy reduction through molecular chain alignment. The newly synthesized SMP has shown the highest recovery stress so far in the literature. Additionally, Li is the first of proposing using two-way SMPs, which expands upon cooling and shrinks upon heating, for sealing joints and cracks in pavement and bridge deck. Furthermore, his group provided the first multiscale modeling for predicting the actuation behavior of twisted-then-coiled polymeric artificial muscle made of fishing lines or two-way SMP fibers. Most recently, his group has synthesized a new 3D printable thermoset polymer integrated with high mechanical strength, shape memory, and recycling capabilities.

As the Associate Vice President at LSU, he is working diligently on STEM education. In addition to advising 34 graduate students to completion, he also directly mentored over 40 undergraduate students on research, and coauthored journal papers with some of them. As PI or Co-PI, he has received 16 education grants from NSF, NIH, Department of Education, etc., with a total funding over $10 million, supporting hundreds of students with scholarships for enhancing their learning experience and career development. He also dedicates his effort on professional service. In addition to review over 600 manuscripts for 124 archival journals and over 130 research proposals for 5 federal funding agencies, he is serving as the Associate Editor: Journals of Materials in Civil Engineering (ASCE), on editorial board: Composites Part B - Engineering (Elsevier), Scientific Reports (Springer Nature), and 4 other journals.

His research, mentoring, and professional services have not gone unnoticed. He has received over 30 awards and recognitions, including “LSU Distinguished Faculty Award,” “Minority Access Faculty Researcher National Role Model Award,” “Society of Plastic Engineers Composite Division Educator of the Year Award,” “ASME Frank Walk Service Award”, etc. His research on spider-silk like SMP fibers, polymeric artificial muscles, self-healing, two-way SMP based sealant, one-way SMP based proppant and expandable cement for loss circulation, etc., have been reported by many news outlets, including Associated Press, Royal Society Chemistry, Materials Today, Air Force Research

Laboratory, MRS Bulletin, American Institute of Physics, American Association for the Advancement of Sciences, Canadian Insider, Society of Plastic Engineers, Louisiana Radio Network, etc.

Some research examples are highlighted below:

(1) G. Li, D. Nettles. *Polymer*, 51(3): 755-762, (2010).

While the current self-healing approaches such as micro-capsules, hollow fibers, thermally reversible covalent bonds, ionomers, incorporation of thermoplastic particles, etc., are very effective in self-healing micro-length scale damage, self-healing of structural scale or macro-length scale damage remains one of the grand challenges facing the self-healing community. We believe that self-healing of structural damage may need multiple steps, at least two steps: close then heal (CTH), similar to the biological healing of wounds in the skin. In a previous study, it has been proven that the confined shape recovery functionality of a shape memory polymer (SMP) based syntactic foam can be utilized to repair structural damage such as impact damage repeatedly, efficiently, and almost autonomously. The purpose of this study is to investigate the effect of various design parameters on the closing efficiencies of both the pure SMP and the SMP based syntactic foam. A systematic test program is implemented, including glass transition temperature (T_g) determination by dynamic mechanical analysis (DMA), isothermal compressive constitutive behavior at various temperatures, and stress-controlled uniaxial compression programming and shape recovery. During thermomechanical cycle testing, two stress levels are utilized for programming and three confinement conditions (fully confined, partially confined, and free) are investigated for shape recovery. It is found that the programming stress is restored under confined recovery conditions, which helps in fully closing the crack; the foam shifts the T_g higher and increases the stiffness at temperatures above the T_g; higher programming stresses lead to slightly higher shape fixity but lower shape recovery in free recovery cases; a higher programming stress also results in a higher peak stress for confined recovery conditions; while the peak stress recovered is controlled by thermal stress, the final stress recovered is controlled by the programming stress, which is stored and recovered using an entropic mechanism. This study lays a solid foundation for using shape memory polymer based composites to self-repair macro-length scale damage.

2) G. Li, W. Xu. *Journal of the Mechanics and Physics of Solids*, 59(6):1231–1250, (2011).

Programming is a key process for thermally activated stress or strain recovery of shape memory polymers (SMPs). Typically, programming requires an initial heating above the glass transition temperature (T_g), subsequent cooling below T_g and removal of the applied load, in order to fix a temporary shape. This work adopted a new approach to program thermoset SMPs directly at temperatures well below T_g, which effectively simplified the shape fixing process. 1-D compression programming below T_g and free shape recovery of a thermoset SMP were experimentally investigated. Functional stability of the shape fixity under various environmental attacks was also experimentally evaluated. A mechanism-based thermoviscoelastic-thermoviscoplastic constitutive model incorporating structural and stress relaxation was then developed to predict the nonlinear shape memory behavior of the SMP trained below T_g. Comparison between the prediction and the experiment showed good agreement. The structure dependence of the thermomechanical behavior of the SMP was further discussed through a parametric study per the validated constitutive

model. This study validates that programming by cold-compression is a viable alternative for thermally responsive thermoset SMPs.

(3) G. Li, A. Shojaei. *Proceedings of the Royal Society A*, 468(2144):2319-2346, (2012).

The difficulty in healing structural damage is that most existing schemes need external help to bring the fractured surfaces in contact before healing can occur. To facilitate the existing schemes to heal macroscopic cracks, we envision that the cracked surfaces can be brought in contact through constrained shape recovery of a shape memory polymer (SMP) fiber reinforced grid skeleton that is embedded in thermoset polymer matrix, similar to stitch a cut in the human skin by suture. In this study, we show that polyurethane SMP fibers can be hardened through cyclic cold-drawing programming, which makes them suitable for reinforcement and healing in thermoset polymer composites. We characterized the microstructure of the SMP fibers, which provides fundamental understanding of the effect of programming on the degree of crystallinity and molecular orientation. Then, a micromechanical multiscale viscoplastic theory is developed to predict the thermomechanical behaviors of the SMP fibers including the cyclic hardening and stress recovery responses. The proposed theory takes into account the stress induced crystallization process and the evolution of the morphological texture based on the applied stresses. The cyclic loading and the thermomechanical responses of the SMP fibers confirm the capabilities of the proposed model in capturing these phenomena.

(4) Q. Yang, G. Li. *Journal of the Mechanics and Physics of Solids*, 92: 237–259, (2016).

A class of innovative artificial muscles made of high-strength polymeric fibers such as fishing lines or sewing threads have been discovered recently. These muscles are fabricated by a simple "twist-insertion" procedure, which have attracted increasing attention due to their low cost and readily availability, giant tensile stroke, record energy density, and easy controllability. In the present paper, we established a multi-scale modeling framework for the thermomechanical actuation responses by a top-down strategy, spanning from macro-scale helical spring analysis down to molecular level chain interaction study. Comparison between modeling results and experimental results exhibited excellent agreement. The effect of the micro-, meso- and macro-scale parameters on the actuation responses of the artificial muscle was further discussed through a parametric study per the validated model. This work helps understand the physical origin behind the remarkable tensile actuation behavior of the twisted-then-coiled polymeric artificial muscles and also provides inspirations for optimal design of advanced artificial muscles made by twist-insertion procedure.

(5) J. Fan, G. Li. *Nature Communications*, 9(1): 642, (2018).

Low output in stress and energy in rubbery state has been a bottleneck for wide-spread applications of thermoset shape memory polymers (SMPs). Traditionally, stress or energy storage in thermoset network is through entropy reduction by mechanical deformation or programming. We here report another mechanism for energy storage, which stores energy primarily through enthalpy increase by stretched bonds during programming. As compared to entropy driven counterparts, which usually have a stable recovery stress from tenths to several MPa and energy output of several tenths MJ/m^3, our rubbery network achieved a recovery stress of 17.0 MPa and energy output of 2.12 MJ/m^3 in bulk form. The giant stress and energy release in the rubbery state will enhance applications of thermoset SMPs in engineering structures and devices.

Delivering Biotech Molecules Without Using Injections

by David J. Brayden, Member EUAS

Short Biography

Professor of Advanced Drug Delivery at University College Dublin (UCD), Ireland Room 231, Veterinary Sciences Centre, UCD Belfield, Dublin 4.

Education

Ph.D. 1989	*Department of Pharmacology, University of Cambridge, UK*
M.Phil. 1988	*Department of Pharmacology, University of Cambridge, UK*
M.Sc. 1986	*Department of Pharmacology, UCD, Ireland*
B.Sc. 1984	*Department of Pharmacology, UCD, Ireland (1st Class Hons.)*

Employment

2014-present	*Full Professor, UCD School of Veterinary Medicine*
2006	*Professor, UCD School of Veterinary Medicine*
2005	*Associate Professor, UCD School of Veterinary Medicine*
2001	*Assistant Lecturer, UCD School of Veterinary Medicine*
1991-2001	*Senior Scientist, Elan Biotechnology Research, Dublin*
1989-1991	*Post-Doctoral Fellow, Cystic Fibrosis Laboratory, Stanford University, CA, USA*

Honours/Awards

1984	*Astra-Zeneca Prize for achieving 1st Place in Finals.*
1985	*Winner of the first Anglo-Irish Scientific Award (British Council) to study for a Ph.D at Cambridge University, UK.*
1994	*Winner of the Sir Patrick Dun Gold Medal for best paper at the Irish National Scientific Medical Meeting (1994)*
1994	*Elected member of the British Pharmacological Society*
1996	*Invited to membership of the New York Academy of Sciences*
1997	*Elected as Fellow of the Royal Academy of Medicine in Ireland*
2001-	*Member of Editorial Advisory Board "Drug Discovery Today"*
2003-2006	*Distinguished Service Awards for Co-chairing the Veterinary Programme at the CRS Annual Meetings (2003-2006)*
2004	*Controlled Release Society-PR Pharmaceuticals Outstanding Veterinary Paper Award*
2005	*Best paper award of the "Journal of Veterinary Pharmacology and Therapeutics"*
2006-2009	*Elected to Board of Scientific Advisors of the Controlled Release Society*
2008	*American Biographical Institute: 'Person of the Year Award in Medicine and Health Care'*
2009	*Distinguished service award from the CRS in recognition for outstanding services on the Board of Scientific Advisors*
2010	*Appointed Associate Editor of "Therapeutic Delivery"*
2012	*American Biographical Institute Hippocrates Award: 'Excellence in the field of medicine'*
2012	*Elected to the College of Fellows of the Controlled Release Society*
2012-	*Biography cited in Marquis Who's Who in Medicine and Healthcare (2012-),Who's Who in Science and Engineering, (2012-), Who's Who in the World (2013-).*
2014	*UCD School of Veterinary Medicine "Outstanding Researcher of the Year Award"*
2014-	*Reappointed to Editorial Advisory Board of Advanced Drug Delivery Reviews*

2015	*Distinguished service award from the CRS Annual Meeting Programme Committee 2015*
	Appointed Adjunct Professor at National University of Ireland, Galway
2016	*Chairman of the Novo-Nordisk Foundation Challenge Programme on "oral drug delivery of biopharmaceuticals"*
2017	*Recipient of Marquis Who's Who® Albert Nelson Lifetime Achievement Award*
2017	*Appointed Senior Associate Editor "Therapeutic Delivery"*
2017	*Lead organiser for the first Keystone Conference on drug delivery (Dublin, 2019)*
2019	*Lead organiser for the first ever Keystone Conference on drug delivery*

David Brayden studies the interaction of biologics with epithelia in order to help design drug dosage forms that cross barriers. Much of the research is on how to convert injectable peptides to oral forms, most recently from the EU FP7 programme, TRANS-INT, to develop nanotechnology to orally deliver insulin and Glucagon-like Peptide 1 (GLP-1). His current research is focussed on how to incorporate intestinal permeation enhancers into solid dosage forms to enable oral delivery of macromolecules. Other strengths are in developing formulations that can be attached to the cheek in order to promote delivery of GLP-1 analogues. This work is part of his role as co-lead Principle Investigator in the Science Foundation Ireland Centre for Medical Devices (2014-2021), which is a national consortium with links to the Medical Device industry. Another project is in the area of intra-articular injection of nanoparticles to offset joint inflammation, work that has been scaled-up for testing in an equine joint lipopolysaccharide model. He also works on oral delivery of food-derived peptide bioactives supplied from the Food industry. The following abstracts are a representative cross-section from his lab's 2018 output.

Selected Publications with abstracts (2018)

1. Bak, A., Ashford, M., & Brayden, D. J. (2018). Local delivery of macromolecules to treat diseases associated with the colon. Adv. Drug Deliv. Rev. 136-137: 2-27. doi.org/10.1016/j.addr.2018.10.009

Current treatments for intestinal diseases including inflammatory bowel diseases, irritable bowel syndrome, and colonic bacterial infections are typically small molecule oral dosage forms designed for systemic delivery. The intestinal permeability hurdle to achieve systemic delivery from oral formulations of macromolecules is challenging, but this drawback can be advantageous if an intestinal region is associated with the disease. There are some promising formulation approaches to release peptides, proteins, antibodies, antisense oligonucleotides, RNA, and probiotics in the colon to enable local delivery and efficacy. We briefly review colonic physiology in relation to the main colon-associated diseases (inflammatory bowel disease, irritable bowel syndrome, infection, and colorectal cancer), along with the impact of colon physiology on dosage form design of macromolecules. We then assess formulation strategies designed to achieve colonic delivery of small molecules and concluded that they can also be applied some extent to macromolecules. We describe examples of formulation strategies in preclinical research aimed at colonic delivery of macromolecules to achieve high local concentration in the lumen, epithelial-, or sub-epithelial tissue, depending on the target, but with the benefit of reduced systemic exposure and toxicity. Finally, the industrial challenges in developing macromolecule formulations for colon-associated diseases are presented, along with a framework for selecting appropriate delivery technologies.

2. Sladek, S., Kearney, C., Crean, D., Brama, P. A. J., Tajber, L., Fawcett, K.,

Labberte, M. C., Leggett, B., & Brayden, D. J. (2018). Intra-articular delivery of a nanocomplex comprising salmon calcitonin, hyaluronic acid, and chitosan using an equine model of joint inflammation. Drug Del. Translational Research, 8 (5) 1421-1435. DOI: 10.1007/s13346-018-0557-x. https://rdcu.be/1ZUk

Polyelectrolyte nanoparticle constructs (NPs) comprising salmon calcitonin (sCT), chitosan (CS), and hyaluronic acid (HA) were previously established as having anti-inflammatory potential when injected via the intra-articular (i.a.) route to a mouse model. We attempted to translate the formulation to a large animal model, the lipopolysaccharide (LPS)-stimulated equine model of joint inflammation. The aim was to manufacture under aseptic conditions to produce sterile pyrogen-free NPs, to confirm physicochemical characteristics, and to test toxicity and efficacy in a pilot study. NP dispersions were successfully formulated using pharmaceutical-grade source materials and were aseptically manufactured under GMP-simulated conditions in a grade A modular aseptic processing workstation. The NP formulation had no detectable pathogen or endotoxin contamination. NPs were then tested versus a lactated Ringer's solution control following single i.a. injections to the radiocarpal joints of two groups of four horses pre-treated with LPS, followed by arthrocentesis at set intervals over 1 week. There was no evidence of treatment-related toxicity over the period. While there were no differences between clinical read-outs of the NP and the control, two synovial fluid-derived biomarkers associated with cartilage turnover revealed a beneficial effect of NPs. In conclusion, NPs comprising well-known materials were manufactured for an equine i.a.-injectable pilot study and yielded no NP-attributable toxicity. Evidence of NP-associated benefit at the level of secondary endpoints was detected as a result of decreases in synovial fluid inflammatory biomarkers.

3. Gleeson, J. G., Frias, J. M, Ryan, S. M., & Brayden, D. J. (2018). Sodium caprate enables the blood pressure-lowering effect of Ile-Pro-Pro and Leu-Lys-Pro in spontaneously hypertensive rats by indirectly overcoming PepT1 inhibition. Eur. J. Pharm. Biopharm 128: 179-187. doi: 10.1016/j.ejpb.2018.04.021.

The tripeptides, Ile-Pro-Pro (IPP) and Leu-Lys-Pro (LKP), inhibit angiotensin-converting enzyme (ACE) resulting in lowered blood pressure. Our hypothesis was that the medium chain fatty acid permeation enhancer, sodium caprate (C10), may prevent the decrease in permeability of the tripeptides when PepT1 is inhibited by glycyl-sarcosine (Gly-Sar), a situation that may occur in the presence of food hydrolysates. Using Caco-2 monolayers and isolated rat jejunal tissue, the apparent permeability coefficients (Papp) of [3H]-IPP and [3H]-LKP were assessed in the presence of Gly-Sar with and without C10. Gly-Sar decreased the Papp of both tripeptides across monolayers and isolated jejunal tissue, but C10 restored it. C10 likely increased the paracellular permeability of the tripeptides, as indicated by immunofluorescence changes in tight junction proteins in Caco-2 monolayers accompanied by a concentration-dependent decrease in transepithelial electrical resistance (TEER). [3H]-IPP and [3H]-LKP were orally-gavaged to normal rats with Gly-Sar, C10, or with a mixture. Plasma levels of both peptides were reduced by Gly-Sar to less than half that of the levels detected in its absence, but were restored when C10 was co-administered. In spontaneously hypertensive rats (SHRs), unlabelled IPP and LKP lowered blood pressure when delivered either by i.v. or oral routes. Oral gavage of Gly-Sar reduced the hypotensive action of peptides in SHRs, but the effect was restored in the presence of C10. In conclusion, there was a reduction in the hypotensive effects of IPP and LKP in SHRs when intestinal PepT1 was inhibited by Gly-Sar, but C10 may circumvent

this by enhancing paracellular permeability.

4. Bhattacharjee, S., Gaspar, M. M., Scholz, D., Almeida, A. J. & Brayden, D. J. (2018). Track-analysis of the passage of rhodamine-labelled liposomes across porcine jejunal mucus in a microchannel device. Therapeutic Delivery 9 (6):419-433. doi: 10.4155/tde-2017-0116.

AIM: To investigate how surface charge and hydrophilicity affect the mucopermeation of liposomes across intestinal mucus. METHODOLOGY: Rhodamine-labeled liposomes (~120-130 nm) with different surface charges were investigated for their capacity to flux across fresh porcine jejunal mucus in a microchannel device. Fluorescent microscopy and tracking analysis were used to measure liposome movement, while fluorescence lifetime imaging microscopy was utilized to determine mucus pH. RESULTS: Mucopermeation was dependent on hydrophilicity and surface charge - anionic liposomes permeated more than cationic. The most cationic liposomal prototype agglomerated mucus. Presence of Na+, K+ and Mg2+ increased both speed and straightness of the pathways for all prototypes. Cationic but not anionic liposomes caused acidification (pH 2.5).CONCLUSION: Acidification caused by cationic liposomes explains their ability to interfere with mucus stability. Surface charge of liposomes strongly influences mucopermeation capability.

5. Heade, J., Maher, S., Bleiel, S. B., & Brayden, D. J. (2018). Labrasol® and salts of medium chain fatty acids can be combined in low concentrations to increase the permeability of a macromolecule marker across isolated rat intestinal mucosae. J. Pharm. Sci. 107: 1648-1655. doi: 10.1016/j.xphs.2018.02.012.

In addition to their solubilizing properties, excipients used in lipid-based formulations can improve intestinal permeability of macromolecules. We determined whether admixing of medium-chain fatty acid (MCFA) permeation enhancers with a lipoidal excipient (Labrasol®) could potentiate transepithelial flux of a poorly permeable macromolecule (fluorescein isothiocyanate dextran 4 kDa [FD4]) across rat intestinal mucosae mounted in Ussing chambers. Low concentrations of sodium caprate (C10), sodium undecylenate (C11:1), or sodium laurate (C12) combined with Labrasol® increased the apparent permeability coefficient (Papp) of FD4 to values typically seen with higher concentrations of MCFAs or Labrasol® alone. For example, combination of C11:1 (0.5 mg/mL) with Labrasol® (1 mg/mL) increased the Papp of FD4 by 10- and 11-fold over the respective individual agents at the same concentrations where no enhancement was evident. The increased enhancement ratios seen with the combinations were associated with some perturbation in intestinal histology and with attenuation of an epithelial functional measure, carbachol-stimulated inward short-circuit current. In conclusion, combining three MCFAs separately with Labrasol® increased the Papp of FD4 to values greater than those seen for MCFAs or Labrasol® alone. Ultimately, this may permit lower concentrations of MCFA to be used in combination with other excipients in oral formulations of poorly permeable molecules.

6. Maher, S., Heade, J., McCartney, F., Waters, S., Bleiel, S. B., Brayden, D. J. (2018). Effects of surfactant-based permeation enhancers on mannitol permeability, histology, and electrogenic ion transport responses in excised rat colonic mucosae. Int. J. Pharmaceutics 539 (1-2):11-22. doi: 10.1016/j.ijpharm.2018.01.008.

Surfactant-based intestinal permeation enhancers (PEs) are constituents of several oral macromolecule formulations in clinical trials. This study examined the interaction of a test panel of surfactant-based PEs with isolated rat colonic mucosae mounted in Ussing chambers in an attempt to determine if increases in transepithelial permeability can be separated from induction of mucosal perturbation. The aim was to assess the effects of PEs on (i) apparent permeability coefficient (Papp) of [^{14}C]-mannitol (ii) histology score and (iii) short-circuit current (ΔIsc) responses to a cholinomimetic (carbachol, CCh). Enhancement ratio increases for Papp values followed the order: C10>C9=C11:1> a bile salt blend>sodium choleate>s ucrose laurate>Labrasol® > C12E8>C12>Cremophor® A25>C7>sucrose stearate>Kolliphor® HS15>Kolliphor® TPGS. Exposures that increased the Papp by ≥2-fold over 120 min were accompanied by histological damage in 94% of tissues, and by a decreased ΔIsc response to CCh in 83%. A degree of separation between the increased Papp of [^{14}C]-mannitol and histological damage and diminution of the ΔIsc response to CCh was observed at selected concentrations of Labrasol®. Overall, this surfactant-based PE selection caused transcellular perturbation at similar concentrations to those that enhanced permeability.

7. Presas, E., McCartney, F., Sultan, E., Hunger, C., Nellen, S., Alvarez, C. V., Werner, U., Bazile, D., Brayden, D. J., O'Driscoll. C. M. (2018). Physicochemical, pharmacokinetic and pharmacodynamic analyses of amphiphilic cyclodextrin-based nanoparticles designed to enhance intestinal delivery of insulin. J. Controlled Release, 286:402-414. DOI: 10.1016/j.jconrel.2018.07.045.

This study describes the rational design, optimization and evaluation of a cyclodextrin-based nanoparticles entrapping insulin glulisine for intestinal administration. A cationic amphiphilic cyclodextrin (click propyl-amine cyclodextrin (CD)) was selected as the primary complexing agent for NP development. Following NP synthesis, in vitro characterization was performed. The insulin glulisine NPs exhibited an average size of 109±9nm, low polydispersity index (0.272) negative zeta potential (-25±3mV), high association efficiency (71.4±3.37%) and an insulin loading of 10.2%. In addition, the NPs exhibited colloidal stability in intestinal-biorelevant media (SIF, supplemented-SIF 1% (w/v) and FaSSIF-V2) for up to 4h. Proteolysis studies indicated that the NPs conferred protection to the entrapped insulin relative to free insulin. In vivo rat jejunal instillation studies demonstrated that the NPs mediated systemic insulin absorption, accompanied by a decrease in blood glucose levels. The relative bioavailability of the instilled insulin (50 IU/kg) from the NP was 5.5% compared to subcutaneous administration of insulin solution (1 IU/kg). The pharmacodynamic and pharmacokinetic data indicate that this cyclodextrin-based formulation may have potential for further research as an oral insulin dosage form.

New Aspects in Biomedical Materials and Clinical Biochemistry

by Pankaj Vadgama, Member EUAS

Short Biography

CURRENT APPOINTMENTS

2000- Director IRC in Biomedical Materials, Queen Mary University of London
2000 - Professor of Clinical Biochemistry, Queen Mary University of London
2000 - 15 Honorary consultant Chemical Pathologist Barts Health NHS Trust
2003 - 15 Head of NHS Clinical Service (Appointed NHS Consultant 1983)
2015- Visiting Professor Southern Medical University Guangzhou, China
2017 - Visiting Professor University of Grenoble Alps

ACADEMIC QUALIFICATIONS

1971 MB, BS Newcastle University
1976 BSc Chemistry (1st Class Hon) Newcastle University
1977 Member (later Fellow) Royal College of Pathologists
1984 PhD Newcastle University
1994 Fellow Royal Society of Chemistry
2001 Fellow Institute of Materials Minerals and Mining
2002 Fellow Institute of Physics
2006 Fellow Royal Society of Medicine
2008 Chartered Scientist (Institute of Materials, Minerals and Mining)
2010 Fellow Royal Society of Biology

ACADEMIC APPOINTMENTS

1977-1980 MRC Training Fellow Newcastle University
1983-1988 Director Biosensor Research Group Newcastle University
1988-2000 Professor of Clinical Biochemistry, Manchester University
1998-2000 Professor of Biomedical Materials, Manchester University
1991-1997 Head of Department of Medicine, Manchester University (Salford)
1993-1996 Postgraduate Dean, Faculty of Medicine, Manchester University
1996-1998 Research Dean, Faculty of Medicine, Manchester University
1998-2000 Head of Division of Biomedical Engineering, Manchester University

Editorial Board Positions

Editorial Board: Physiological Measurement, Medical Engineering and Physics, Bioanalytical Reviews, Functional Biomaterials, Medical Devices and Sensors, 3D Printed Systems and Materials, Journal of Biochemistry and Molecular Biology Research, Chinese Chemical Letters. Guest Editor for Analytical and Bioanalytical Chemistry: (i) Thin film characterisation (ii) Membrane based sensors. Sub-Editor Biomaterials Series (RSC). Editor for (i) Bioelectrochemistry for the Encyclopedia of Interfacial Chemistry, Surface Science and Electrochemistry (ii) Bioinstrumentation and Bioinformatics for the Encyclopedia of Biomedical Engineering (Elsevier).

National/International Committees

Member EPSRC (Engineering and Physical Science Research Council): Materials Strategic Advisory Team (SAT) (2004/5/7/8); Healthcare (2005). Member, Institute of Materials Minerals and Mining Smart Materials Committee, Nanotechnology Committee, Biomedical Applications Division and External Advisory Committee. National Measurement Systems (NMS) Grants Committees for Materials and Modelling (2002 – 15) and Innovation R&D (2012-15); NPL(National Physical Laboratory)/LGC (Laboratory of the Government Chermist) projects. Past EPSRC grants panel memberships (includes as chair of some panels) from 1986: Materials, Structural Materials, Chemistry, Multidisciplinary (Engineering), Health Care, Analytical Science, Mechanical and Medical Engineering, Follow-on Funding, DTCs (Doctoral Training Centres), Master's Training

Packages, Sensors' Policy Group, SMART Technologies, Basic Sciences, Life Science Interface, Engineering Fellowships (Senior/Advanced). Nanotechnology Strategy Working Group (co-author, section on nanomedicine) (2005). ROPA (Realising our Potential) Panels EPSRC, MRC (Medical Research Council) (1995-96). MRC Joint Research Equipment Initiative Panel (JREI, 1996-7). Royal Society of Chemistry, Industrially-Sponsored Award in Electroanalytical Chemistry (1997, 2000). Member of Organisation and Delivery of Healthcare Task Force (Foresight Healthcare, 1999-2000). Member Academy of Medical Sciences/Foresight Working Group on the Detection and Identification of Infectious Disease (2004). Member Institution of Electrical Engineers Professional Group S9 (Biomedical Engineering, 1990-93). Chair (i) R&D (ii) Point of Care Testing committees, Division of Pathology Barts Health NHS Trust (2002-2011). Member BBSRC Strategic Research Studentships Panel 2004, LINK Program Medical Technologies and Molecular Sensors (1994-2001), Foresight LINK awards (2001). European Space Agency Advisory Panel on bioassay under microgravity (2000). Various EU FP IV & V Panels: Biotechnology, Biomedical and Health Research, Cell Factory, Growth, Standards, Measurements and Testing (1993-2000). Chair DTI Building up Biomaterials (BuB) Materials Healthcare Advisory Group (2001-2003). Member UK delegations (x3) to Japan (Biomaterials) and Singapore (x1) (Materials). Roadmap Champion for Diagnostics for human health, RSC (2010). Member Manchester Commonwealth Games 2002 Scientific Congress Committee.

RAE (Research Assessment Exercise, UK) Panel member Materials (2008). External Assessor Faculty of Engineering, University of Coimbra, Portugal (2013), Founder member biennial international conference series: Biomaterials Interfaces (2007-). Chair RSC Chemistry in Medicine Panel (2010). Chair, Steering Committee EPSRC IRColl Interdisciplinary Research Collaboration) in Bionanotechnology, University of Oxford (2003-5), Member 4th Generation Light Source (4GLS) Advisory Group, Daresbury. Member, international task force on environmental carcinogens (Halifax Project, 2014). Advisor, UK Biobank Project (2004). Member Special Inquiry into Regenerative Medicine Research at UCL.

RAE Advisor University of Manchester, REF Advisor University of Central Lancashire. Academic promotions advisor (Rutgers, Cranfield, Ulster, Manchester, Leeds, Flanders). Advisor, Engineering – Materials Faculty research quality, Limerick (2011). Cranfield University Senate committee panel member on Biomedicine MScs (2013). External advisor on the reorganization of the Chemistry Department, University of Surrey (2001). Scrutineer for Fellowship/Membership applications to the Institute of Materials Minerals and Mining. External assessor for staff appointments, PhD applications for Nazarbayev University (2014). Advisor to University of Ege (Turkey) on summer school biotechnology rolling Programme. International advisory member (vice-chair) of Uganda based research training foundation; advice on training needs and external funding, eg secured for geological sciences MScs. Co-Chair UK – China Biomaterials Partnership (2006-9). Global Initiative of Academic Networks (GIAN, India)) lecture course at University of Tezpur (2016). Host to Commonwealth Fellows India (Tezpur, 2015; Aligarh Muslim University, 2003), PhD Fellow (Government of Pakistan, 2017). NMS research project advisor, LGC (2005-07).

Chair UK Foresight Panel on Biomaterials and member of Materials, Smart Materials panel (2004) (co-author, strategy documents). Member, DTI Innovation and Growth Team (2006), Member UK Standards Group on ISO TC 229; nanotechnology nomenclature (2006 -). Chair of ISO Working Group on Nanomedicine and member Working Group on Nanobiotechnology (2006 – 2010). Member BSI Committees on Nanotechnology, Botechnology and Cell Therapies.

Member DFG Review Panel for German Excellence Initiative: Materials 2005,2007). Member Finland Research Council panel on Bioscience and Engineering (2008). Grants reviewing national funding councils: Australia, Quatar, Hong Kong, Portugal, Austria, Netherlands, Italy, Ukraine, Kazakhstan, Netherlands, Romania.

RECENT COLLABORATIONS

-EPSRC Program grant on elite athlete monitoring (ESPRIT) with Loughborough University Imperial College and UK Sport (£600k) (2011-15)

-DoH Dual function nano-silver incorporated polymers for medical device antimicrobial coatings – 2 projects (total £263 k) (2010 – 2014) Rainbow Medical Ltd

-EU Marie Curie exchange with five China Universities: Microsystems and Bioanalysis Platforms for Health Care (£78k) (2010 – 14)
-Industrial CASE Studentship on polymer bioadhesives with UEA, TWI (2012 -16)
-EU Marie Curie exchange with three China Universities Advanced biomaterials for generative medicine (£39k) (2010 – 15)
-UKIERI collaboration with Central Electronics Engineering Research Institute, India on Micro/nanofluidics for diagnostics (£65k) (2014 -16).
-TSB/BBSRC grant on Blood brain barrier model for drug permeability and toxicity testing with Kirkstall Ltd and Leeds University. (£52k) (2014-15)
- DoH Anti-bacterial 'Fill & Flush' Urinary Catheter Development with University of Southampton (£61k) (2017 -19)
- Newton Institutional Links Grant (Egypt) Renewable Energy Driven Hybrid Desalination System for Remote Areas (£115, 647) (2016 – 18)

Abstracts 2018

Challenges for successful implantation of biofuel cells

There is a growing interest in the design and engineering of operational biofuel cells that can be implanted. This review highlights the recent progress in the electrochemistry of biofuel cell technologies, but with a particular emphasis on the medical and physiological aspects that impact the biocompatibility of biofuel cells operating inside a living body. We discuss the challenge of supplying power to implantable medical devices, with regard to the limitations of lithium battery technology and why implantable biofuel cells can be a promising alternative to provide the levels of power required for medical devices. In addition to the challenge of designing a biofuel cell that provides a stable level of sufficient power, the review highlights the biocompatibility and biofouling problems of implanting a biofuel cell that have a major impact on the availability of the substrates inside body that provide fuel for the biofuel cell. These physiological challenges and associated ethical considerations are essential to consider for biofuel cells that are designed to be implanted for long-term operation inside a living animal and eventually to human clinical applications.

Bifunctional aptamer-mediated catalytic hairpin assembly for the sensitive and homogenous detection of rare cancer cells

The presence of cancer cells in body fluids confirms the occurrence of metastasis and guides treatment. A simple, fast, and homogeneous fluorescent method was developed to detect cancer cells based on catalytic hairpin assembly (CHA) and bifunctional aptamers. The bifunctional aptamer had a recognition domain for binding to target cancer cells and an initiator domain for triggering the CHA reaction. In the presence of target cells, the bifunctional aptamer was released from the inhibitor and initiated a cascade reaction of assembly and disassembly of the hairpins. Separation of the fluorophores from the quenchers produced fluorescence signals. The proposed strategy showed high specificity for discriminating normal cells and leukocytes, and the detection limit was 10 cells/mL, which was lower than that of previous aptasensors. This assay was further tested using four kinds of clinical samples spiked with target cells to confirm its applicability. We developed a simple, rapid, and cost-effective method for the detection of cancer cells that did not require purification, and the approach holds great potential for bioanalysis and early diagnosis.

High temporal resolution delayed analysis of clinical microdialysate streams

This paper presents the use of tubing to store clinical microdialysis samples for delayed analysis with high temporal resolution, offering an alternative to traditional discrete offline microdialysis sampling. Samples stored in this way were found to be stable for up to 72 days at - 80 degrees C. Examples of how this methodology can be applied to glucose and lactate measurement in a wide range of in vivo monitoring experiments are presented. This paper presents a general model, which allows for an informed choice of tubing parameters for a given storage time and flow rate avoiding high back pressure, which would otherwise cause the microdialysis probe to leak, while maximising temporal resolution.

New directions in membrane designs for biosensors

For practical outcomes, to avoid cumbersome and undesirable sample preparation, biosensors require engineered sample interfacing to control the dynamics of exchange at the sensing surface. This is a particular priority for biomedical biosensors, given the diversity of cellular and macromolecular sample constituents capable of disrupting not only the transduction sequence, but also of passivating the vulnerable sensing surface. Polymeric, and to a lesser extent inorganic membranes offer the most effective of the available technologies for this. This review covers the most recent work in this area, and through this provides indication of new directions and the consolidation of existing ones. The growing need to deliver advanced materials solutions for operational biosensors is likely to accelerate future development in this adjunct area

Bayesian Graphical Games for Synchronization in Dynamical Networks

by Frank Lewis, Member EUAS

Short Biography

Dr. Lewis was born in Würzburg, Germany, subsequently studying in Chile and Gordonstoun School in Scotland. He obtained the Bachelor's Degree in Physics/Electrical Engineering and the Master's of Electrical Engineering Degree at Rice University in 1971. He spent six years in the U.S. Navy, serving as Navigator aboard the frigate USS Trippe (FF-1075), and Executive Officer and Acting Commanding Officer aboard USS Salinan (ATF-161). In 1977 he received the Master's of Science in Aeronautical Engineering from the University of West Florida. In 1981 he obtained the Ph.D. degree at The Georgia Institute of Technology in Atlanta, where he was employed as a professor from 1981 to 1990. He is Moncrief-O'Donnell Endowed Chair Professor of Electrical Engineering at The University of Texas at Arlington.

Member, National Academy of Inventors. Fellow of the IEEE, Fellow of IFAC, Fellow of the U.K. Institute of Measurement & Control, Fellow American Association for the Advancement of Sciences, Member of the New York Academy of Sciences. Registered Professional Engineer in the State of Texas and Chartered Engineer, U.K. Engineering Council. Ranked at position 85 worldwide, 64 in the USA, and 3 in Texas of all scientists in Computer Science and Electronics, by Guide2Research (October 2018). Qian Ren Thousand Talents Consulting Professor, Northeastern University, Shenyang, China. Charter Member (2004) of the UTA Academy of Distinguished Scholars. UTA Academy of Distinguished Teachers 2012. IEEE Control Systems Society Distinguished Lecturer 2012-1014. Founding Member of the Board of Governors of the Mediterranean Control Association. Served as Visiting Professor at Democritus University in Greece, Hong Kong University of Science and Technology, Chinese University of Hong Kong, City University of Hong Kong, National University of Singapore, Nanyang Technological University Singapore. Distinguished Foreign Scholar, Nanjing Univ. Science & Technology. Project 111 Professor at Northeastern University, China. Elected Guest Consulting Professor at Shanghai Jiao Tong University and South China University of Technology.

Received IEEE Computational Intelligence Society Neural Networks Pioneer Award 2012, AIAA Intelligent Systems Award 2016, John Ragazzini Education Award 2018 from American Automatic Control Council. Received Fulbright Research Award 1988, American Society of Engineering Education F.E. Terman Award 1989, Int. Neural Network Soc. Gabor Award 2009, U.K. Inst Measurement & Control Honeywell Field Engineering Medal 2009, three Sigma Xi Research Awards, UTA Halliburton Engineering Research Award, UTA Distinguished Research Award, ARRI Patent Awards, various Best Paper Awards, IEEE Control Systems Society Best Chapter Award (as Founding Chairman of DFW Chapter), and National Sigma Xi Award for Outstanding Chapter (as President of UTA Chapter). Received Outstanding Service Award from the Dallas IEEE Section and selected as Engineer of the year by Ft. Worth IEEE Section. Listed in Ft. Worth Business Press Top 200 Leaders in Manufacturing. Appointed to NAE Committee on Space Station in 1995 and IEEE Control Systems Society Board of Governors in 1996. Received the 2010 IEEE Region 5 Outstanding Engineering Educator Award and the 2010 UTA Graduate Dean's Excellence in Doctoral Mentoring Award. Texas Regents Outstanding Teaching Award 2013.

Current interests include intelligent control, distributed cooperative control on graphs, nonlinear systems, reinforcement learning, process control, and neurobiological systems. 47,000 google citations, h-index 97. Author of 7 U.S. patents, 376 journal papers, 52 chapters and encyclopedia articles, 420 refereed conference papers, and 20 books including Optimal Control, Optimal Estimation, Applied Optimal Control and Estimation, Aircraft Control and Simulation, Control of Robot Manipulators, Neural Network Control, High-Level Feedback Control with Neural Networks and the IEEE reprint volume Robot Control. Editor of Taylor & Francis Book Series on Automation & Control Engineering. Served as Editor for the flagship journal Automatica. Served/serves on many Editorial Boards including International Journal of Control, Neural Computing and Applications, Optimal Control & Methods, and Int. J. Intelligent Control Systems. Recipient of NSF Research Initiation Grant and continuously funded by NSF since 1982. Since 1991 he has received $8 million in

funding from NSF, ARO, ONR, AFOSR and other government agencies, including significant DoD SBIR and industry funding. His SBIR program was instrumental in ARRI's receipt of the US SBA Tibbets Award in 1996.

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Bayesian Graphical Games for Synchronization in Dynamical Networks

Victor G. Lopez, Yan Wan, Senior Member, IEEE, and Frank L. Lewis, *Fellow, IEEE*

IEEE TRANSACTIONS ON CONTROL OF NETWORK SYSTEMS, VOL.X, NO.X

In this paper, differential games with incomplete information, or Bayesian games, are formulated for multiagent continuous-time dynamical systems in a communication graph. These new Bayesian graphical games represent the situation where the agents are uncertain about their actual payoff functions and must employ the evidence observed from the behavior of other agents to improve their estimation of the real setting of their environment. Furthermore, the agents play their best response strategies with respect to the policies of their neighbors defined by the graph topology. A tight relationship between the beliefs of an agent and his distributed best response control policy is established. Conditions for the so-called Bayes-Nash equilibrium are provided for such games with linear dynamics and general cost functions. Two belief update algorithms are proposed for the agents to review their strategies using information obtained from the graph topology.

Conclusion

Multiagent systems analysis was performed for dynamical agents engaged on interactions with uncertain objectives. We reveal for the first time the tight relationship between the beliefs of an agent and his distributed best response control policy. The Bayes-Nash equilibrium were proved for the best response control policy to achieve under general conditions. The proposed naïve likelihood approximation is a useful method to deal with the limited knowledge of the agents about the graph topology, provided that its restrictive assumptions do not excessively differ from the actual game environment.

Simulations with two different belief update algorithms show the applicability of the proposed methods. The Bayesian belief update has the advantage of not requiring an additional communication scheme, achieving convergence of the beliefs using solely measurements of the states of their neighbors. The non-Bayesian updates take advantage of a supplementary information to achieve a faster and more robust convergence of the beliefs to the true type of the game.

Optimal and Autonomous Control Using Reinforcement Learning: A Survey

This paper reviews the current state of the art on reinforcement learning (RL) based feedback control solutions to optimal regulation and tracking of single and multi-agent systems. Existing RL solutions to both optimal H_2 and H_∞ control problems, as well as graphical games will be reviewed. RL methods learn the solution to optimal control and

game problems online and using measured data along the system trajectories. We discuss Q-learning and integral reinforcement learning (IRL) algorithm as core algorithms for discrete-time (DT) and continuous-time (CT) systems, respectively. Moreover, we discuss a new direction of o -policy RL for both CT and DT systems. Finally, we review several applications.

Conclusion and open research directions

In this paper, we have reviewed several RL techniques for solving optimal control problems in real time using data measured along the system trajectories. We have presented families of online RL-based solutions for optimal regulation, optimal tracking, Nash and graphical games. The complete dynamics of the systems do not need to be known for these RL-based online solution techniques. As another approach to speed up the learning by reuse of data, experience replay technique used in RL was discussed. These algorithms are fast and data efficient because of reuse of the data for learning.

The design of static RL-based output-feedback controllers for nonlinear systems has not been investigated yet. Also existing RL-based H_8 controllers require the disturbance to be measured during learning. Another interesting and important open research direction is to develop novel deep RL approaches for feedback control of nonlinear systems with high-dimensional in-puts and unstructured input data. Deep neural networks (DNNs) can approximate a more accurate structure of the value function and avoid divergence of the RL algorithm and consequently instability of the feedback control system. Deep RL for feedback control, how-ever, require developing new learning algorithms that assure the stability of the feedback system in the sense of Lyapunov during the learning.

Traffic Theory and Modelling for Smart Urban Mobility Systems

by Xiaobo Qu, Member EUAS

Short Biography

Xiaobo Qu obtained his PhD, Master's degree, and Bachelor's degree from National University of Singapore, Tsinghua University, and Jilin University, respectively. He is now a professor and chair of urban mobility systems in the Department of Architecture and Civil Engineering, Chalmers University of Technology in Sweden. Before his professorial appointment at Chalmers, he served as a faculty member at the Griffith University and the University of Technology Sydney, where he holds adjunct professorship now. Throughout his academic career, he has been endeavouring to practically improve transport safety, efficiency, equity, and sustainability through traffic flow modelling, network optimisation, and most recently emerging technologies. He has authored or co-authored over 80 journal articles published at top tier journals in the area of transport engineering, and he is a recipient of prestigious Ministry of Transport (Singapore) Minister's Innovation Award, President Graduate Fellowship, and Australian Department of Education and Training Endeavour Cheung Kong research fellowship. His research has been supported by Australian Research Council Discovery Programme, Queensland Department of Transport and Main Roads, Transport for New South Wales, Sydney Trains, Australian Department of Education and Training, National Natural Science Foundation of China, Swedish Innovation Agency Vinnova, and European Union. He is currently an area/associate/guest editor for several leading journals including IEEE Transactions on Cybernetics, IEEE Intelligent Transport Systems Magazine, ASCE Journal of Transportation Engineering Part A: Systems, ASCE ASME Journal of Risk and Uncertainty in Engineering Systems, Applied Energy, Computer Aided Civil and Infrastructure Engineering, and the Chair of Traffic Theory and Modelling Special Interest Group of World Congress for Transport Research Society.

Urban mobility challenges (safety, congestion, sustainability, etc.) significantly undermine a large city's liveability and the wellbeing of its residents: i) traffic crashes result in over 1.25 million fatalities and 50 million injuries worldwide annually; ii) gridlocks/congestion occur more and more frequently in our urban cities, especially during peak hours; and iii) the transport sector contributes 1/3 of the greenhouse gas emissions (World Health Organization, 2014).

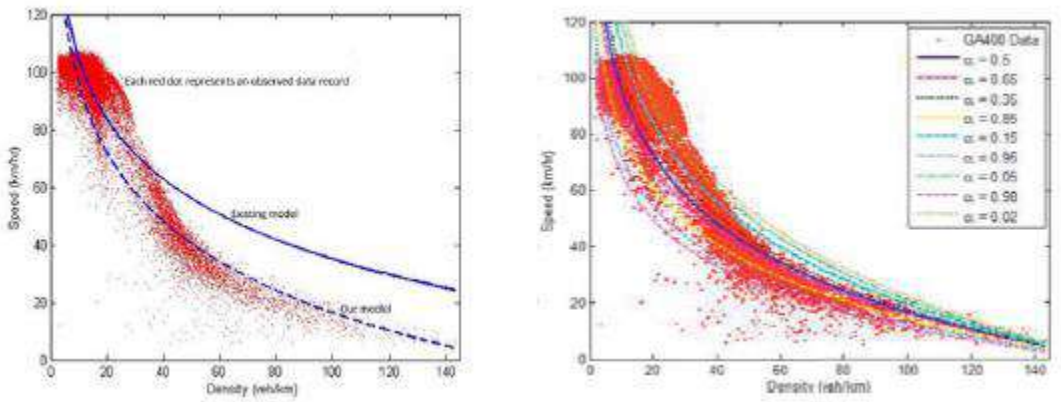
Modern urban mobility systems have been transforming rapidly in recent years, ranging from individual vehicle technologies to system level management. On the one hand, a series of vehicle technology innovations have blossomed in the past couple of decades, just to name a few, connected vehicles, self-driving cars, electric vehicles, Hyperloop, and even flying cars. They may radically change behaviours and mechanisms of not only individual transportation elements but also a whole transportation system. On the other hand, transportation system operations are experiencing a paradigm shift from infrastructure-based traffic management into individual-traveller-cantered mobility services, such as car sharing, ridesharing, and on-demand services. These innovations and breakthroughs have motivated researchers on Intelligent Transportation Systems (ITS) to expand the frontiers

of ITS concepts and skillsets, to identify new opportunities and challenges in integrating emerging vehicle technologies and mobility services, and to produce theories, models, field experiments and real world applications for establishing a unique ITS discipline. In the above-mentioned areas of smart urban mobility systems, Professor Xiaobo Qu and his collaborators have made contributions to the following important areas:

1. Traffic flow theory

- Traffic flow fundamental diagram, as the name suggested, is the foundation for traffic engineering discipline. It has been long time that researchers endeavour to find a continuous and differentiable closed form to consistently represent traffic flow fundamental diagram. However, these efforts have been unsuccessful and most scholars compromise to use equations without a closed form. We realised that the inaccuracy is caused by not only functional forms but also sample selection bias (Qu et al., 2015, Zhang et al., 2018). Based on this observation, we propose a new calibration approach to perfectly resolve the above-mentioned problem. As can be seen in Figure 1(a), the model can represent traffic flow consistently well ranging from free flow conditions to traffic jam conditions.

- Based on the above study, we apply a new calibration approach to generate stochastic traffic flow fundamental diagrams (Qu et al., 2017). We first prove that the percentile based fundamental diagrams are obtainable based on the proposed model. We further prove the proposed model has continuity, differentiability and convexity properties so that it can be easily solved. A sample of stochastic fundamental diagram is shown in Figure 1(b). This proposed methodology has wide applications in the connected era by considering flow stochasticity.



(a) deterministic diagram (b) stochastic diagram

Figure 1: Traffic flow fundamental diagram

- We propose a novel model to define and estimate a traffic flow vulnerability (Kuang et

al., 2015). By imposing a hypothetical disturbance to the leading vehicle, the following vehicle's action is represented as a probabilistic causal model. After that, a tree is built to describe the eight possible conflict types under the model. A corresponding surrogate measure, named Aggregated Crash Index (ACI), is thus proposed to measure the crash risk. This index reflects the accommodability of freeway traffic state to a traffic disturbance.

2. Traffic operations and control

- We improve the capacity estimation model in Highway Capacity Manual for roundabouts (Qu et al., 2014). According to solid field data, the errors have been narrowed from around 12% to 5%. This achievement has been applied by many transport agencies in different countries.

- We propose a novel and practical concept for freeway traffic management: long-distance commuter (LDC) lane (Qu and Wang, 2015). The LDC lane is a dedicated lane that only long distance commuters can use. Since there is only minor disturbance from forced lane-changing of vehicles from other lanes, the LDC lane admits a much higher capacity. Our preliminary study demonstrates that LDC lane significantly increases speed as well as overall capacity.

- We apply the traditional user equilibrium and road pricing concept to long distance commuting public transit system (Wang and Qu, 2017). Based upon this, we design the optimal fare structure that can improve the efficiency of transit system as a whole. We further develop a trial and error pricing scheme that is able to shorten the headways of trains by reducing the dwell time (Wang et al., 2018).

3. Modelling mixed traffic of connected and automated vehicles

- We have done a series of works in this area including simulation, optimisation, learning design, and experimental design. We first propose a simulation based approach to improve the merging capacity and alleviate traffic oscillations by introducing a collaborative scheme (Zhou et al., 2017). Then we propose a centralised approach based on optimisation model to control/regulate vehicle speeds with an aim of vehicle and infrastructure integration. Both exact and heuristic approaches are designed to solve the above model (Li et al., 2018). In order to improve the computational efficiency, we further design learning based approach in order to take into account the historical experiences and beneficial practice. Please refer to Figure 2 for the safety, efficiency, and sustainability benefits for an example of mixed traffic flow.

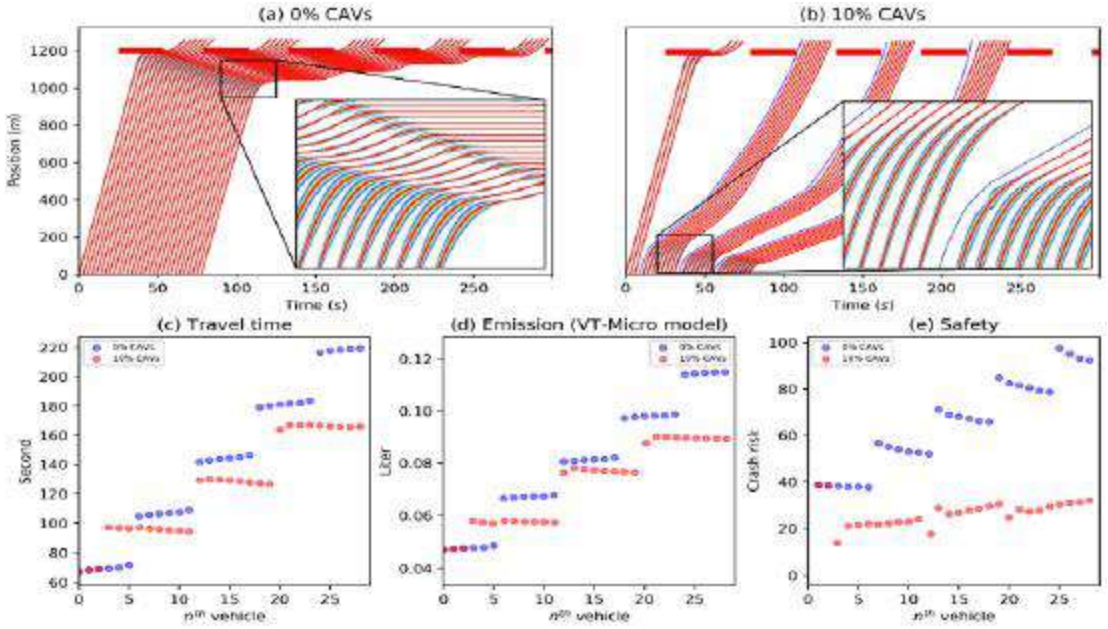


Figure 2: An example of mixed traffic flow

- We propose a recurrent neural network based microscopic car following model that is able to accurately capture and predict traffic oscillation. An appropriate structure and objective function are designed in order to re-establish traffic oscillations and distinguish driver's characteristics. The model takes into account both global and local information in the decision making process and is able to formulate mixed traffic flow for future traffic.

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Kuang, Y., Qu, X., and S. Wang, 2015. A tree-structured crash surrogate measure for freeways. *Accident Analysis and Prevention*, 77, 137-148.

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Zhou, M., Qu, X., and Li, X., 2017. A recurrent neural network based microscopic car following model to predict traffic oscillation. *Transportation Research Part C*. 84, 245-264.

Investigation on a New Cellular Structure, the 'Porosome'

by Bhanu P. Jena, Member EUAS

Short Biography

I was born in Jajpur, a small town in Odisha, India, on November 1, 1955, to Manju and Prafulla Jena. My early childhood was spent in remote villages in Odisha, where my grandfather Braja Kishore practiced medicine. The dedication of my father and grandfather to science and medicine and their service to humanity greatly influenced me to choose a career in science. I majored in Chemistry, Zoology, and Botany, for my Undergraduate studies at BJB College in Bhubaneswar, Odisha (B.Sc., 1975) and completed a Master's Degree in Zoology (Endocrinology) from Utkal University, (M.Sc., 1978). I graduated top of my graduating class in the Masters of Science program and received the Prasant Ku. Memorial Prize and the Utkal University Gold Medal. In December of 1988, I received Doctorate Degree (Ph.D.) in Zoology (Molecular Endocrinology), and the Research Excellence Award from Iowa State University. Following postdoctoral training as a Fellow at Yale University, I accepted a faculty appointment at Yale University as an Assistant Professor, and in 2000, moved to the Department of Physiology, at Wayne State University School of Medicine, as a tenured full Professor, and Founder-Director of the Institute of NanoBioScience. In 2004, I was conferred the title of Distinguished Professor, and the George E. Palade University Professor by the Board of Governors of Wayne State University. I am the only living University Professor, and the second at Wayne State University's 150-year history. Since high school, my passion has been to understand the workings of the unit of life, 'the cell'. At a very early age, I was fascinated by the complexity of 'the cell' in electron micrographs, similar to the complexity of a city, yet every aspect of its function is so precisely regulated. My scientific enquiry on how cells secrete, led to the discovery of the "porosome" -a new cellular structure and a molecular nanomachine, demonstrated to be the universal secretory portal in cells involved in the fractional release of intra-vesicular contents during secretion. Currently, the major focus of my laboratory is to determine the distribution of proteins within the porosome complex using single particle cryoelectron microscopy, and small angle x-ray solution and neutron scattering. Additionally, in the past 15 years, I have been involved in institution building to bring the benefits of science and education to society.

Among the honors and awards I have received over the years are: 2015 Distinguished Scientist Award from the Society for Experimental Biology and Medicine; Elected Foreign Member of the Georgian National Academy of Science; Fellow AAAS; Elected Foreign Member of the Korea Academy of Science & Technology; Elected Foreign Member of the

National Academy of Medicine, Romania; Elected Member of the EU Academy of Science; the Swebelius Cancer Research Award; the Hallim Distinguished Award Lecture jointly with the Prof. Ahmed H. Zewail; Sir. Aaron Klug Award; ASAS Basic Biological Science Award; Ranbaxy Basic Research in Medical Sciences Award; George E. Palade Gold Medal; elected to the Academy of Scholars at Wayne State University; six Honorary Doctorates including one from Babes-Bolyai University, Romania, jointly with Professors George E. Palade and Günter Blobel; and Distinguished Visiting Professorships in a number of academic institutions. Throughout my career, I have been very fortunate to avail the opportunity to learn from wonderful teachers and scholars, and to work with students and colleagues with a passion for science. My family has been a great source of peace, inspiration, and joy in life.

Professional Memberships and Activities

1988-	*Member, American Association for the Advancement of Science*
1988-	*Full Member of Sigma Xi Scientific Society*
1990-	*Member of the American Society for Cell Biology*
2000-	*Member of the American Physiological Society*
2012-	*Member of the Society for Experimental Biology and Medicine*
2014-	*Member of the American Chemical Society*
2002-	*Foreign Member, Korean Academy of Science and Technology.*
2005-	*Foreign Member National Academy of Medical Sciences, Romania*
2011-	*Fellow, American Association for the Advancement of Science*
2012-	*Foreign Member of the Georgian National Academy of Science*
2018-	*Foreign Member of the European Union Academy of Science*

Honors

1976	*National Merit Scholarship Awarded by the Government of India.*
1978	*Utkal University Prasant Ku. Memorial Prize for outstanding scholastic achievement*
1978	*Utkal University Scholastic Merit Gold Medal*
1988	*Iowa State University Humanitarian Award*
1988	*Iowa State University Research Excellence Award*
1992 & 1993	*Twice recipient of the Swebelius Cancer Research Award*
1995 & 1996	*Twice recipient of the OHSE Award, Yale University*
2002	*Wise & Hellen Burroughs Foundation Lecture*
2002	*Doctor Honoris Causa, Vasile Goldis University, Romania*
2002	*Distinguished Visiting Professor, Vasile Goldis University, Romania*
2002	*Elected Foreign Member, Korean Academy of Science and Technology*
2002	*Honorary Doctor of Philosophy, Pusan National University, Korea.*
2002	*Distinguished Visiting Professor, Pusan National University, Korea.*
2002	*Hallim Award, Korean Academy of Science and Technology, jointly with the late Prof. Ahmed H. Zewail.*
2003	*Doctor Honoris Causa, "Iuliu Hatieganu" University of Medicine & Pharmacy, Romania.*
2003	*Honorary Doctorate, 'Babes-Bolyai' University, Romania, May 26, 2003, jointly with the late Prof. George E. Palade, and Prof. Günter Blobel.*
2003	*Distinguished Visiting Professor, 'Babes-Bolyai' University, Romania, May 26, 2003.*
2003	*Honorary Doctorate, Institute of Physiology, Georgian Academy of Sciences, Georgia*
2004	*Distinguished Professor, Wayne State University*
2004	*George E. Palade University Professor, Wayne State University*
2005	*Sir Aaron Klug Award*
2005	*Honorary Doctorate in Medicine, 'Carol Davila' University, Bucharest, Romania*
2005	*George E. Palade Distinguished Lecture & Medal, Wayne State University School of Medicine.*
2006	*Felicitation & Award, Maharashtra Association for Cultivation of Science, Pune, India*

2006	*Distinguished Visiting Professor, Agharkar Research Institute, Govt. of India, Pune, India*
2006	*Elected Foreign Member National Academy of Medical Sciences, Romania*
2006	*G. E. Palade Distinction Medal for excellence in medicine, 'Carol Davila' University, Bucharest, Romania*
2007	*Elected to the Academy of Scholars, Wayne State University*
2007	*American Society of Animal Science, 'Basic Biological Science Award'*
2009	*Ranbaxy Basic Research in Medical Sciences Award*
2011	*Fellow, American Association for the Advancement of Science*
2012	*Foreign Member Georgian National Academy of Science*
2014	*Honorary Professor, University of Medicine & Pharmacy of Tirgu Mures, Romania*
2015	*"2015 Distinguished Scientist Award", Society for Experimental Biology and Medicine, USA*
2017	*Honorary Life-time Professor, Delhi University, India*
2017	*Honorary Scientist, Victor Babes National Research Institute, Romania*
2018-	*Foreign Member of the European Union Academy of Science*

Over 22 years ago, our laboratory made the fundamental discovery of a new cellular structure the 'porosome', and since has elucidated its morphology, composition, function as the universal secretory portal in cells, and its functional reconstitution in lipid membrane and in live cells.

Porosomes are cup-shaped supramolecular lipoprotein structures at the cell plasma membrane ranging in size from 15 nm in neurons and astrocytes, to 100-180 nm in endocrine and exocrine cells. Neuronal porosomes are composed of nearly 40 proteins, including a number of integral membrane proteins. The controlled release of secretory products governed by porosomes, represent one of the central mechanisms through which cells communicate with the outside world, central to cellular function. Secretory defects in cells are associated with many diseases including diabetes, cystic fibrosis, digestive, as well as neurological, and immune disorders. The porosome discovery has brought about a paradigm-shift in our fundamental understanding of the secretory process in cells, with the promise of improved management and treatment of a plethora of diseases resulting from secretory defects.

Secretion is a fundamental cellular process in living organisms, from yeast to cells in humans. Secretion is both responsible and required for a variety of physiological activities, such as neurotransmission and the release of hormones and digestive enzymes. Correspondingly, secretory defects in cells are responsible for a host of debilitating diseases. Since the mid 1950's, it was believed that secretory vesicles completely merged with the cell plasma membrane during secretion, resulting in release of the entire vesicular contents. While this provides one mechanism for secretion, the observation of partially empty vesicles in cells following secretion is incompatible with complete vesicle merger, suggesting the presence of an additional mechanism that allows partial discharge of intra-vesicular contents during secretion.

In the mid 1990's, motivated by the goal of identifying cellular structures at the plasma membrane involved in the regulated fractional release of intravesicular contents from cells, we employed the then newly developed technique of atomic force microscopy (AFM) to image the morphology and dynamics of the live pancreatic acinar cell surface at the nanometer scale during secretion. The major breakthrough came in 1996, when circular pit-like structures containing 100-180 nm depressions or pores were observed at the apical plasma membrane of pancreatic acinar cells, where secretion is known to occur. During secretion, the depressions or pores grew larger, returning to their resting size following

completion of cell secretion. We first reported these results on January 1, 1997 in the Proceedings of the National Academy of Sciences (PNAS 94:316-321). The next breakthrough was communicated by a succession of papers by our research team, with the results establishing these observed depressions to be the secretory portals at the plasma membrane in cells. In January 2002 and February 2003, we reported in two studies, one in Cell Biology International and the other in Biophysical Journal, that following stimulation of cell secretion, gold-conjugated amylase antibodies (amylase being one of the major intravesicular enzymes secreted by pancreatic acinar cells) accumulate at these depressions. These results established the depressions to be the long sought-after secretory portals in cells. The study reported in the Biophysical Journal, further demonstrated the presence of t-SNAREs at the porosome base facing the cytosol, firmly establishing the depression structures to be secretory portals where vesicles transiently dock and fuse for intravesicular content release during secretion. In March 2002, Jena, reported in the journal Endocrinology on the depressions and their dynamics at the cell plasma membrane in growth hormone (GH) secreting cells of the pituitary gland, and on the accumulation of GH-immuno-gold at depressions following secretion. In the same year in a separate study, Jena reported the depression structure and their dynamics in chromaffin cells. In September 2003 following isolation of these structures from acinar cells of the exocrine pancreas, our laboratory finally determined their composition and functionally reconstituted the isolated structures into artificial lipid membranes, reported in the Biophysical Journal. In the same study, morphological details of the structure associated with docked secretory vesicle, were revealed using electron microscopy. In the 20 years following the initial observation of these membrane structures, by employing a combination of approaches such as AFM, biochemistry, electrophysiology, conventional EM, mass spectrometry, and X-ray solution scattering analysis, Jena discovered these structures to be present in all secretory cells examined, including, perhaps most significantly, neurons. His studies established this new supramolecular lipoprotein structure at the cell plasma membrane to be secretory portals that performs the specialized function of fractional discharge of intravesicular contents from cells during secretion. This specialized structure was named by Jena the ‘porosome’. The discovery of the porosome has overturned traditional views on how cells secrete. Finally, in 2016, isolated porosomes from beta cells of the endocrine pancreas were functionally reconstituted in live beta cells, establishing its critical function as the universal secretory machinery in cells and promise in therapy.

The significance of the identification of the porosome is reflected by the great number of publications on porosomes and associated transient fusion mechanism accompanied by fractional discharge of intravesicular contents from cells. As a consequence, “secretory granules are recaptured largely intact following stimulated exocytosis in cultured endocrine cells” [PNAS. 2003, 100:2070-2075]; “single synaptic vesicles fuse transiently and successively without loss of identity” [Nature 2003, 423:643-647]; and “zymogen granule exocytosis is characterized by long fusion pore openings and preservation of vesicle lipid identity” [PNAS 2004, 101:6774-6779].

Air Breathing Engines - Gas Turbine Heat Transfer, Cooling, and Aerodynamics

by Phil Ligrani, Member EUAS

Short Biography

Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, Propulsion Research Center, 5000 Technology Drive, University of Alabama at Huntsville

PROFESSIONAL PREPARATION

University of Texas at Austin	*Mechanical Engineering*	*Bachelor of Science, 1974*
Stanford University	*Mechanical Engineering*	*Master of Science, 1975*
Stanford University	*Mechanical Engineering*	*Doctor of Philosophy, 1980*

APPOINTMENTS

2014 – present	*Eminent Scholar in Propulsion, Professor of Mechanical and Aerospace Engineering, Department of Mechanical and Aerospace Engineering, University of Alabama*
2010 – 2014	*Professor of Aerospace & Mechanical Eng, Saint Louis University*
2010 – 2013	*Director of Graduate Programs, Parks College, Saint Louis University*
2006 – 2009	*Statutory Professor, Department of Engineering Science, University of Oxford*
2006 – 2009	*Director, Rolls-Royce UTC (University Technology Centre)*
1997 – 2006	*Professor, Department of Mechanical Engineering, University of Utah*
2002 – 2006	*Adjunct Professor, Department of Bioengineering, University of Utah*
1992 – 1997	*Associate Professor, Department of Mechanical Engineering, University of Utah*

ARCHIVAL JOURNAL PUBLICATIONS AND RELATED ITEMS.

As of December 2018, Dr. Ligrani is author or co-author of more than 184 publications in archival journals, including the International Journal of Heat and Mass Transfer, the ASME Transactions-Journal of Turbomachinery, the ASME Transactions-Journal of Engineering for Gas Turbines and Power, the ASME Transactions-Journal of Heat Transfer, the ASME Transactions-Journal of Fluids Engineering, the Journal of Fluid Mechanics, the AIAA Journal, Experiments in Fluids, Physics of Fluids, the AIAA Journal of Heat Transfer and Thermophysics, the International Journal of Rotating Machinery, Separation Science and Technology, Sensors and Actuators A: Physical, and the Journal of Microcolumn Separations. He is also author of 9 book chapters, and about 138 conference presentations and publications. A number of these are invited conference presentations at international meetings, at locations which include Korea, France, the Ukraine, Croatia, Germany, England-United Kingdom, and Belgium. From 1994 to 2018, he has also presented approximately 180 lectures at different institutions and establishments, including many invited lectures. From 2010 to 2018, he presented 4 Invited Keynote Papers, 7 Invited Papers, and 7 Invited Plenary Keynote Papers at different international conferences. Current SCOPUS Reference Citation H-INDEX is 40. Current GOOGLE SCHOLAR Reference Citation H-INDEX is 44.

EDITOR ACTIVITIES.

From 1998 to 2000, Dr. Ligrani served as Guest Editor for a Special Topical Issue for Measurement Science and Technology. He has also served as Associate Editor for the ASME Transactions-Journal of Heat Transfer from 2003 to 2006, and from 2010 to 2014, and as Associate Editor for the ASME Transactions-Journal of Fluids Engineering from 2005 to 2008. Present editor duties include: (i) Member of the Distinguished Editorial Review Board for the Advances in Transport Phenomena, Book Series with Springer Publishing Corporation (since 2006), (ii) Editorial Board Member, Power and Thermal Engineering Processes and Equipment Journal, Published by the National Technical University "Kharkov Polytechnic Institute", Russia and Ukraine (since 2015), (iii) Editorial Board Member, International Journal of Innovative Works in Engineering and Technology (IJIWET) (since 2015), (iv) Associate Editor, Journal of Propulsion Technology (JPT) Journal, Published by CNPIEC, P. R. China (since 2015), (v) International Editorial Board Member, Industrial Thermal Engineering Journal, Published by Thermogasdynamics Department, National Academy of Sciences of Ukraine, Kiev, Ukraine (since 2018), (vi) Editorial Board Member, Advances in Aerodynamics (AIA) Journal. Published by the Chinese Society of Aerodynamics (CSA), and the China Aerodynamics Research and Development Center (CARDC), P. R. China (since 2018), (vii) Associate Editor, Energies Journal (since 2018), (viii) Associate Editor, ASME Transactions-Journal of Journal of Engineering for Gas Turbines and Power (2018-2021).

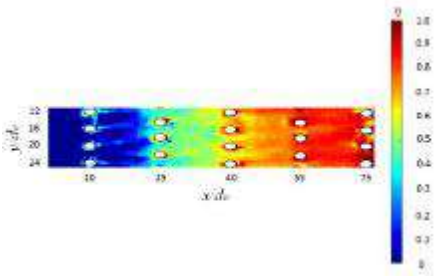
SELECTED RECENT HONORS, AWARDS, ACADEMIC RECOGNITIONS

● Outstanding Mechanical Engineer of the Year Award 2016, ASME – American Society of Mechanical Engineers, NAS - North Alabama Section, USA. ● Distinguished Advisory Professor, Inje University, South Korea, 2010 to 2020. ● Distinguished Lecture Award, 2011, CEAS Distinguished Lecture Series, College of Engineering, University of Wisconsin, Milwaukee, Wisconsin, USA. ● Distinguished Editorial Review Board membership for Springer Publishing Corporation. ● Carl E. and Jessie W. Menneken Faculty Award for Excellence in Scientific Research. ● NASA Space Act Tech Brief Award for "Development of Subminiature Multi-Sensor Hot-Wire Probes." ● Silver Winner for the Annual 26th Educational Advertising Awards for the Higher Education Marketing Report.

Dr. Ligrani has a strong past and present record of working with many different collaborators and co-workers, from many locations throughout the world. Additional information on selected, currently active research projects is provided within sections which follow. **(i) Traditional Heat Transfer and Fluid Mechanics Investigations** involving electronics cooling, heat transfer augmentation, drag reduction, turbulent boundary layers, flows in channels with dimpled surfaces, flows in curved channels, elastic turbulence, slot impingement cooling, and macro-scale pumps and pump flows. Also included are **aerodynamics investigations with *high-speed, compressible flows at transonic and supersonic Mach numbers***, including SWBLI – Shock Wave Boundary Layer Interactions. Related projects involve **transonic and supersonic experimental testing**. Research interests also include experimental diagnostics in high speed flows, and air breathing propulsion. **(ii) Air Breathing Engines - Gas Turbine Heat Transfer, Cooling, and Aerodynamics Losses**, including internal cooling, film cooling, impingement cooling, cooling of extremities, aerodynamic performance including aerodynamic losses, and transonic turbine flows and heat transfer. This subject area includes the effects of uses of bio-fuels, synthetic fuels, and renewable energy sources in relation to gas turbines and gas turbine heat transfer and cooling technologies. Note that an important area of turbomachinery research interest involves heat transfer and aerodynamics investigations with *high-speed, compressible flows at transonic and supersonic Mach numbers*, including linear cascade studies. **(iii) Micro-Fluidics and Millimeter-Scale-Fluidics**, including micro-pump flows, and the effects of slip phenomena on gas and liquid flows in micro-scale passage flows with and without surface roughness, including the effects of hydrophobic surfaces and elastic turbulence. **(iv) Experimental Techniques**, including development of millimeter-scale multiple-hole pressure probes, subminiature hot-wire anemometry, and infrared thermography.

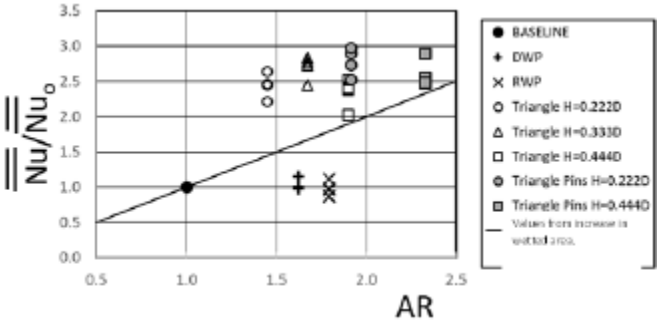
DOUBLE WALL COOLING RESEARCH INVESTIGATIONS

Provided are new effusion cooling data for both surfaces of full coverage effusion cooling plate. For the effusion cooled surface, measured are spatially-resolved distributions of surface adiabatic film cooling effectiveness, and surface heat transfer coefficients (measured using transient techniques and infrared thermography). For the impingement cooled surface, measured are spatially-resolved distributions of surface Nusselt numbers (measured using steady-state liquid crystal thermography). To produce this cool side augmentation, impingement jet arrays at different jet Reynolds numbers, from 2720 to 11100, are employed. Experimental data are given for a sparse effusion hole array, with spanwise and streamwise impingement hole spacing such that coolant jet hole centerlines are located midway between individual effusion hole entrances. Considered are initial effusion blowing ratios from 3.3 to 7.5. The velocity of the freestream flow which is adjacent to the effusion cooled boundary layer is increasing with streamwise distance, due to a favorable streamwise pressure gradient. Such variations are provided by a main flow passage contraction ratio CR of 4. Overall, the present results show that, for the same main flow Reynolds number, approximate initial blowing ratio, and streamwise location, significantly increased thermal protection is generally provided when the effusion coolant is provided by an array of impingement cooling jets, compared to a cross flow coolant supply. An example of hot-side surface, local adiabatic film cooling effectiveness variation (measured using infrared thermography) for an initial blowing ratio of 7.5 and a mainstream Reynolds number of 147000 is presented within the attached figure.



IMPINGEMENT JET ARRAY COOLING RESEARCH USING TARGET SURFACES WITH SPECIAL TEXTURES AND SURFACE ROUGHNESS DISTRIBUTIONS

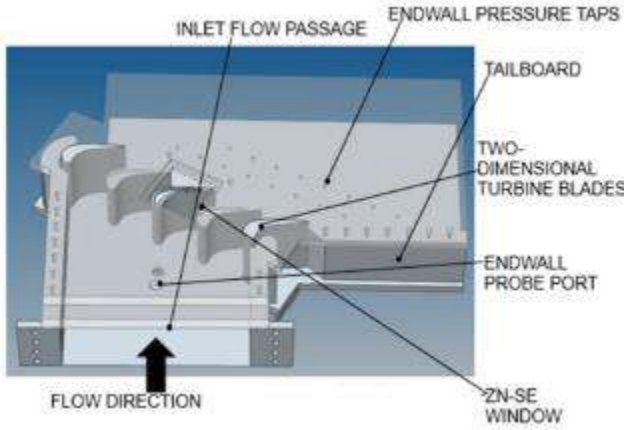
The target surface experimental results are obtained with target surfaces with a variety of different surface roughness and surface texture arrangements. One arrangement employs arrays of small triangle roughness elements, with different roughness heights, both with and without the addition of large pin roughness elements. The impingement plate employed contains round holes, such that holes in adjacent streamwise rows are staggered with respect to each other. As such, data are provided for different impingement jet Reynolds numbers (based on impingement jet hole diameter) of 900, 1500, 5000, and 11000. Resulting variations in performance are then related to different roughness element arrangements, with different ratios of wetted surface area to flat projected area, as well as to target surface internal conduction, and to the increased three-dimensional transport and mixing produced by arrays of target surface roughness elements. Shown within the attached figure are Nusselt number ratio values as dependent upon AR, ratio of wetted surface area to flat baseline area, wherein configurations with different surface roughness arrangements are compared for impingement jet Reynolds numbers of approximately 11000. Note that the values associated with solid line are associated with an increase in wetted surface area. Within the figure, data are given for different magnitudes of roughness height H, where impingement hole diameter is denoted D.



TURBINE BLADE HEAT TRANSFER RESEARCH WITH INNOVATIVE FILM COOLING CONFIGURATIONS

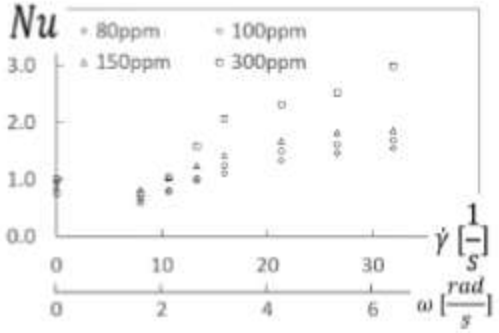
Currently, there is a deficit of experimental data for surface heat transfer characteristics and thermal transport processes associated with tip gap flows, and a lack of understanding of performance and behavior of film cooling as applied to blade tip surfaces. As a result, many avenues of opportunity exist for development of creative tip configurations with innovative external cooling arrangements. Overall goals of the present investigations are to reduce cooling air requirements, and reduce thermal loading, with equivalent improvements of thermal protection and structural integrity. Of interest is development of a two-dimensional linear cascade with appropriate cascade airfoil flow periodicity. Included are boundary layer flow bleed devices, downstream tailboards, and augmented cascade inlet turbulence intensity. The present linear cascade approach allows experimental configuration parameters to be readily varied. Tip gap magnitudes are scaled so that ratios of tip gap to inlet boundary layer thickness, ratios of tip gap to blade axial chord length, and ratios of tip gap magnitudes to blade true chord length match engine hardware configurations. Ratios of inlet boundary layer thickness to tip gap range from 3 to 5. Innovative film cooling configurations are utilized for one blade tip configuration, and scaled engine components are modelled and tested with complete external cooling arrangements. Blade tip

and geometry characteristics are also considered, including squealer depth and squealer tip wall thickness. Results are obtained with engine representative transonic Mach numbers, Reynolds numbers, and film cooling parameters, including density ratios, which are achieved using foreign gas injection with carbon dioxide. Transient, infrared thermography approaches are employed to measure spatially-resolved distributions of surface heat transfer coefficients, adiabatic surface temperature, and adiabatic film cooling effectiveness. Presented within the attached figure is a three-dimensional view of the turbine blade cascade which is employed for the investigation.



THERMAL TRANSPORT ENHANCEMENT FROM ELASTIC TURBULENCE

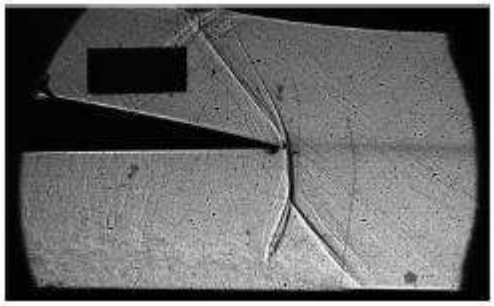
The influences of elastic turbulence on convective heat transfer, within a rotating Couette flow arrangement are experimentally determined using viscoelastic fluids, and Boger fluids, which are constant viscosity solvents. Different concentrations of polyacrylamide in 65 percent sucrose solutions are used, along with solutions with 65 percent sucrose only, as different magnitudes of shear stress and strain rate are imposed upon the flow field. Transition and development of elastic turbulence are characterized, along with convective heat transfer enhancements. The resulting increased levels of mixing, transport, and diffusion from elastic turbulence give convective heat transfer coefficient enhancements which are as large as 240 percent, relative to Boger fluids at the same shear rate, rotation speed, flow passage height, and flow temperature. Variations of spectra of static temperature fluctuations, and mean-square magnitudes of fluctuating static temperature provide evidence of increased flow irregularities and unsteadiness (relative to Boger solution flows), which are believed to result from elastic turbulence induced polymer twisting, unsteadiness, and convolutions. Shown within the attached figure are Nusselt number variations with shear rate and disk rotational speed for different polymer concentrations (ppm), for the 2/3 radial location within the rotating Couette flow environment.



INVESTIGATIONS OF SHOCK WAVE UNSTEADINESS

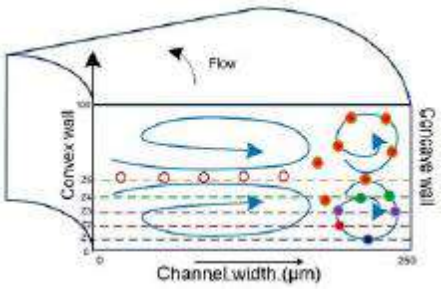
Despite over fifty years of research on shock-wave-boundary-layer-interaction unsteadiness, the source, origin, and propagation direction of the unsteadiness remains controversial and a debated topic. The present research effort is designed to address normal shock wave unsteadiness characteristics, using a newly-developed, supersonic wind tunnel, which is located at the University of Alabama in Huntsville, USA. The wind tunnel test section includes a two flow passage arrangement, where each passage is separated by a shock wave holding plate. The top wall for the

top passage is contoured relative to the streamwise flow direction, and a choking flap is located at the downstream portion of the bottom flow passage. With this arrangement, the Mach number at the test section inlet is 1.54, and total air mass flow rate is approximately 12.5 kg/s. Of particular interest are spatially- and temporally-varying flow structural characteristics, which are quantified using shadowgraph flow visualization images, grayscale value spectral energy variations, magnitude squared coherence variations with frequency, and time lag magnitude variations with frequency, where these last two quantities are determined for different flow locations relative to shock wave locations. Two-point correlation functions, as they vary with frequency, indicate that perturbations at a Strouhal number Str of 0.0144 originate downstream of the shock wave and propagate upstream. At a Strouhal number Str of 0.0057, perturbations originate near the shock wave and propagate both upstream and downstream. Coherence functions, determined between different flow locations within the present investigation, show strong correlation between the shock wave and the downstream boundary layer exists at Str = 0.0029. Overall results thus demonstrate that perturbations associated with unsteadiness do not all originate in the same location, nor travel in the same direction. The attached figure shows a shadowgraph flow visualization image from recent research efforts, which illustrates the presence of a normal shock wave, lambda foot, and separated turbulent boundary layer within the lower flow passage, and an oblique shock wave system within the upper flow passage. Note that flow direction is from right to left.



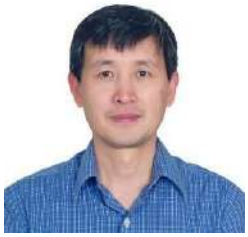
DEAN FLOW DYNAMICS IN LOW-ASPECT RATIO SPIRAL MICROCHANNELS

A wide range of microfluidic cell-sorting devices has emerged in recent years, based on both passive and active methods of separation. Curvilinear channel geometries are often used in these systems, due to presence of secondary flows, which can provide high throughput and sorting efficiency. Most of these devices have been designed on the assumption that there are two counter rotating Dean vortices, present in the curved rectangular channels, which exist in the state of steady rotation and amplitude. Investigated are associated secondary flows in low aspect ratio spiral rectangular microchannels, in order to define their development with respect to the channel aspect ratio and Dean number. This work is the first to experimentally and numerically investigate Dean flows in microchannels for *Re* > 100, and show presence of secondary Dean vortices beyond a critical Dean number. Also demonstrated is the impact of these multiple vortices (>2) on particle and cell focusing. Ultimately, this work offers new insights into secondary flow instabilities for low-aspect ratio, spiral microchannels, with improved flow models for design of more precise and efficient microfluidic devices for applications such as cell sorting and micromixing. The included figure shows a schematic diagram of the positions where the confocal images were taken to determine the position of trapped 10 µm particles.



Novel Numerical Methods for Singularly Perturbed and Degenerate PDEs and PDE constrained Optimisation Problems in Classic and Financial Engineering

by Song Wang, Member EUAS



Short Biography

Professor Song Wang, born in 1958 in Wuhan, China, received a B.Sc. degree in Applied Mathematics from Wuhan University of Hydraulic and Electric Engineering, Wuhan (now Wuhan University) in 1982 and a Ph.D. in Numerical Analysis from Trinity College Dublin in 1989, under the supervision of Professor John Miller. Upon his PhD graduation, he was employed by a Dublin-based hi-tech company Tritech Ltd as a senior software engineer and then the technical director. During the period of 1989 to 1992, he managed and was a main contributor to a number of research projects from the then EEC.

In late 1992, he migrated from Ireland to Australia to take up a research position at the University of New South Wales. He was then employed by Curtin University of Technology as a lecturer in 1995. From 1999 to 2014 he was an academic in the School of Mathematics & Statistics, The University of Western Australia (UWA), where he got promoted to senior lecturer, associate professor and professor. He also served as the Deputy Head of School at UWA in 2013. In 2014 he moved to Curtin University as a professor of computational mathematics and Head of Dept. of Maths & Stats. Currently he is the Head of Discipline of Mathematics & Statistics, Curtin University.

In addition to his regular positions in Australia, has held visiting or adjunct professor positions at various overseas universities such as HK Polytechnic University, National Sun Yat-sen University, Sichuan Normal University, Tianjin University of Finance & Economics and Wuhan University. His also a distinguished visiting professor of Laboratory for General Applied Mathematics, Northeast Normal University China, and a director of the China-Australia Collaboration in Applied Optimization, a research centre jointly by Federation University, Curtin University, Shanghai University and Chongqing Normal University.

Professor Wang's research interests include scientific computation, numerical optimization and optimal control, optimum design and computational finance. He is a world-leading researcher in these areas and has published many research papers, mostly in well-established international journals. His research activities have been supported financially by government organisations and private sectors from Australia, China, Hong Kong and US. He has supervised numerous PhD students to completion and delivered plenary and keynote talks at many international conferences and workshops. Currently, he is on the editorial boards of several international journals. Below is a list of snap-shots of his research achievements.

Fitted finite volume method for the degenerate Black-Scholes equation

A novel numerical method for a degenerate partial differential equation, called the Black-Scholes equation, governing financial option pricing was developed by him. The method is based on a fitted finite volume spatial discretization and an implicit time stepping technique. To derive the error bounds for the spatial discretization of the method, he formulates it as a Petrov-Galerkin finite element method with each basis function of the trial space being determined by a set of two-point boundary value problems defined on element edges. Stability of the discretization is proved and an error bound for the spatial discretization is established. It is also shown that the system matrix from the discretization is an *M*-matrix so that the discrete maximum principle is satisfied by the discretization. Numerical experiments are performed to demonstrate the effectiveness and usefulness of the method.

Based on the above work, a super-convergent finite-volume method is also developed for the non-linear Black-Scholes' equation. Unlike conventional finite volume methods in which the dual mesh points are naively chosen to be the midpoints of the subintervals of the primal mesh, we construct the dual mesh judiciously using an error representation for the flux interpolation so that both the approximate flux and solution have the second-order accuracy at the mesh points without any increase in computational costs. As the equation is degenerate, we also show that it is essential to refine the meshes locally near the degenerate point in order to maintain the second-order accuracy. Numerical results for both European and American options with constant and non-constant coefficients will be presented to demonstrate the super-convergence of the method.

Penalty method for complementarity problems (or Hamilton-Jacobi-Bellman equations) arising in financial engineering

Most of problem arising in financial engineering, particularly those from pricing financial options are Hamilton-Jacobi-Bellman (HJB) equations of the form:

$$\min\{L_1 v - f_1, L_2 v - f_2, \ldots, L_M v - f_M\} = 0$$

in a domain Ω and time interval $[0,T]$ with terminal and boundary conditions, where L_1 is a 2nd-order differential operator, $L_2,\ldots,L_M$ are the 1st or 0th order operators, and $f_1,\ldots,f_M$ are given functions. This is equation is normally non-linear and non-smooth. In our early work, we developed a power penalty function approach to the differential linear and non-linear complementarity problems arising from pricing European and American options of various types. Such a problem is first reformulated as a variational inequality, and the resulting variational inequality is then approximated by a nonlinear parabolic partial differential equation with a power penalty term. It is shown that the solution to the penalized equation converges to that of the variational inequality problem with an arbitrary order. This arbitrary order convergence rate allows one to achieve the required accuracy of the solution to a problem with a small penalty parameter. A numerical scheme for solving penalized nonlinear partial differential equations is also proposed. Numerical results are given to illustrate the theoretical findings and to show the effectiveness.

Penalty methods for various types of linear and non-linear HJB equations of the above form in finite dimensions arising from the discretization of infinite-dimensional HJB equation of the above form have also developed and analysed. These includes both exterior and interior penalty methods. For each of the numerical methods developed, we have established a convergence theory. Numerical results show that our method provide very

efficient and useful tools for solving HJB equations of practical significance.

Novel numerical methods for HJB equations governing optimal feedback control

Using a dynamic programming approach, an optimal feedback control problem in engineering can be written as the following form.

$$-\frac{\partial V}{\partial x} + sup_{u\in U}\left[-\nabla V \cdot f\big(t, x(t), u(t)\big) - L(t, x(t), u(t))\right] = 0$$

for $(x, t) \in R^n \times (0,1)$ subject to some given terminal conditions, where x and u are respectively state and control, U is a given set of feasible controls and f and L are given functions.

Numerical solution of the above HJB equation often incurs the so called 'curse of dimensionality' problem as the problem is usually in high spatial dimensions. We have designed several efficient numerical methods for solving this HJB equation. These include Radial Basis Function (RBF) based (mesh-less) numerical methods, RBF methods with an adaptive technique for generating RBF spaces, and a domain decomposition technique along with the RBF method. Numerical results show that our method can solve the above HJB equation in moderate dimensions. Thus, our methods provide an efficient tool for constructing feedback control laws for real-world optimal feedback control problems. We have also designed and analysed several mesh-based numerical methods for solving the HJB equation in up to 3-dimenmsional space. All these methods have made HJB equations of practical importance computationally more tractable.

Numerical solution of singularly perturbed convection-diffusion equations

We have formulated and analysed various finite volume and (mixed) finite element methods for singularly perturbed convection-diffusion equations including the semiconductor device equations of the drift-diffusion model and Navier-Stockes equations. We have shown that these methods are stable for all range of the singular perturbation parameters involved. In particular, our numerical methods for solving semiconductor device equations have been featured in a survey paper published by *Reports on Progress in Physics* (1999) and a chapter in one of the '*Handbook of Numerical Analysis*' series (2005). Our exponentially fitted finite volume method for singularly perturbed advection-diffusion equations has been the foundation for solving HJB equations mentioned above.

Representative significant publications

1. J.J.H. Miller, S. Wang, A New Non-conforming Petrov-Galerkin Finite Element Method with Triangular Elements for a Singularly Perturbed Advection-Diffusion Problem, *IMA J. Numer. Anal*., **14** (1994) 257—276.
2. J.J.H. Miller, S. Wang, A Tetrahedral Mixed Finite Element Method for the Stationary Semiconductor Continuity Equations, *SIAM J. Numer. Anal.*, **31**, No.1, (1994) 196—216.
3. S. Wang, A novel exponentially fitted triangular finite element method for an advection-diffusion problem with boundary layers, *J. Comput. Phys*., **134** (1997) 253-260.
4. J.J.H. Miller, W.H.A. Schilders, S. Wang, Application of finite element methods to the simulation of semiconductor devices, *Reports on Progress in Physics*, **63**, No.3 (1999) 277-352.
5. J.J.H. Miller, E. O'Riordan, G.I. Shishkin, S. Wang, Parameter robust Schwartz method for a singularly perturbed reaction-diffusion problem with an interior layer, *Appl Numer Math*, **53** (2000) 323-337.
6. W.R. Lee, S. Wang, K.L. Teo, An optimization approach to a finite dimensional parameter estimation problem in semiconductor device design", *J. Comput. Phys*., **156**, No.2 (1999) 241—256
7. S. Wang. Z.C. Li. A Non-Conforming Combination of the Finite Element and Volume Methods for a Singularly Perturbed Convection-Diffusion Equation, *Math. Comput,* Vol.72, No.244 (2003) 1689-1709.

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Multiscale Multiphase Heat and Mass Transfer

by Yuwen Zhang, Member EUAS

Short Biography

Professor Mechanical and Aerospace Engineering (MAE) Department University of Missouri (MU) Columbia, Missouri, USA

Education

Ph.D., Mechanical Engineering, University of Connecticut, Storrs, CT, 1998
D.Eng., Engineering Thermophysics, Xi'an Jiaotong University, Xi'an, China, 1991
M.Eng., Engineering Thermophysics, Xi'an Jiaotong University, Xi'an, China, 1988
B.Eng., Thermal Turbomachinery, Xi'an Jiaotong University, Xi'an, China, 1985

Experience

2009– Professor, MAE Department, MU
2013–2017 Department Chair, MAE Department, MU
2003–2009 Associate Professor, MAE Department, MU
2001–2003 Assistant Professor, Department of Mechanical Engineering, New Mexico State University (NMSU), Las Cruces, New Mexico
2000–2000 Senior Engineer, Thermoflow, Inc., Sudbury, Massachusetts
1995–2000 Research Scientist/Associate, Department of Mechanical Engineering, University of Connecticut, Storrs, Connecticut
1994–1995 Research Associate, Department of Mechanical and Materials Engineering, Wright State University, Dayton, Ohio
1991–1994 Assistant Professor, School of Energy and Power Engineering, Xi'an Jiaotong University (XJTU), Xi'an, Shaanxi, China
1985–1991 Research/Teaching Assistant, School of Energy and Power Engineering, XJTU

Awards and Honors

Member, EU Academy of Sciences (EUAS), 2018–
Coulter Award, University of Missouri Coulter Translational Partnership Program, 2018
Fellow, American Association for the Advancement of Sciences (AAAS), 2015–
Certificate of Appr. for Service as K-15 Committee Chair, ASME Heat Transfer Division, 2014
James C. Dowell Professorship, College of Engineering, MU, 2012–2018
Certificate of Distinguished Service, American Inst. of Aeronautics and Astronautics (AIAA), 2011
Chancellor's Award for Outstanding Research and Creative Activity, MU, 2010
Missouri Honor Senior Faculty Research Award, College of Engineering, MU, 2010
Associate Fellow, American Institute of Aeronautics and Astronautics (AIAA), 2008–
Fellow, American Society of Mechanical Engineers (ASME), 2007–
Faculty Fellow, College of Engineering, MU, 2007–2012
Computational Research Award, Department of Mechanical Engineering, NMSU, 2003
Young Investigator Award, U.S. Office of Naval Research (ONR), 2002
Dissertation Fellowship Award, University of Connecticut Research Foundation, 1998
Summer Fellowship Award, University of Connecticut Research Foundation, 1997, 1998
First Class Scientific Achievement Award, XJTU, 1992, 1993

Membership at Professional Societies
Fellow, American Association for the Advancement of Science (AAAS), 2015 –
Fellow, American Society of Mechanical Engineers (ASME), 2007 –
Associate Fellow, American Institute of Aeronautics and Astronautics (AIAA), 2008 –
Member, American Society for Engineering Education (ASEE), 2001 –
Member, American Society of Thermal and Fluids Engineers (ASTFE), 2015 –
Member, American Physical Society (APS), 2016 –
Member, World Academy of Science, Engineering and Technology (WASET), 2017 –
Editorial Positions
Co-Editor-in-Chief, Frontiers in Heat and Mass Transfer, 2010–
Associate Editor, ASME Journal of Heat Transfer, 2017–
Associate Editor, Journal of Fluid Flow, Heat and Mass Transfer, 2017–
Associate Editor, Journal of Advances in Mechanical Engineering and Sciences (JAMES), 2014–
Editorial Board Member, Chinese Journal of Aeronautics (CJA), 2013–
Editorial Board Member, Journal of Xi'an Jiaotong University, 2011–
Editorial Board Member, Journal of Electronics Cooling and Thermal Control, 2011–
Editorial Board Member, Pioneer Journal of Heat and Mass Transfer and its Applications, 2010–
Co-Editor-in-Chief, Frontiers in Heat Pipes, 2010–2017
Associate Editor (Engineering), IARS' International Research Journal, 2012–2015
Editorial Board Member, Journal of Advanced Thermal Science Research, 2014–2017
Editorial Board Member, International Scholarly Research Notices, 2011–2017
Editorial Board Member, ISRN Thermodynamics, 2011-2014
Editorial Board Member, ISRN Mechanical Engineering, 2010–2014
Editorial Advisory Board Member, The Open Thermodynamics Journal, 2008–2013

His research area is in the field of thermal and fluid sciences with applications in manufacturing, thermal management, and energy systems. He has actively led research activities sponsored by federal funding agencies including the Office of Naval Research (ONR), the Air Force Research Laboratory (AFRL), the U.S. Army Program Executive Office, and the National Science Foundation (NSF). He has co-authored three textbooks [1-3] and edited four books in the field of thermal and fluids sciences and engineering. He has published over 300 papers in top journals as well as more than 180 papers in national and international conferences. His publications have been cited over 7500 times and his h-index is 42. His most significant contributions are summarized below:

- He has made significant contributions across a wide spectrum of thermal and fluids science and engineering. He has developed pioneer models for a latent heat thermal energy storage system, which is very important for applications of clean energy [4, 5]. With support of the ONR and NSF, he has developed a series of multiscale, multiphysics models on Additive Manufacturing (AM), including Selective Laser Sintering (SLS) and Laser Chemical Vapor Deposition/Infiltration (LCVD/LCVI) [6, 7]. The common characteristics of these technologies is that heat transfer cannot be analyzed by simple and traditional models because of several complicated thermal and fluids processes that are occurring simultaneously. He is the first to develop a very innovative model to simulate fluid flow and heat transfer within an oscillating heat pipe [8, 9], which is a heat transfer device that can be used in cooling for electronic devices and thermal management of life support systems. His research in these areas is documented in three books [1-3].
- He is also aggressively pursuing research activities in ultrafast, ultra-intense laser interaction with materials for applications in nanomanufacturing, which is an interdisciplinary research field that involves physics, chemistry, mechanical

engineering and laser technology. With laser- pulse durations of one quadrillionth of a second, femtosecond lasers are poised to change the way research is done in a variety of disciplines in science, engineering and medicine. He has developed multiphysics models that describe femtosecond laser interaction with metal and biological materials ranging from molecular scales to larger system levels [10, 11].

- His group has also carried out a Molecular Dynamics (MD) simulation to reveal the mechanism of heat transfer enhancement in nanofluids which are stable colloidal suspensions of solid nanomaterials with sizes typically on the order of 1-100 nm in the base fluid [12, 13]. His recent research is in the area of thermal management and temperature uniformity improvement of Li-ion batteries using external and internal cooling methods [14, 15]. His group proposed to utilize pin fin heat-sinks and metal/non-metal foams, as well as using electrolyte flow inside the embedded microchannels in the porous electrodes as a novel internal cooling technique. These achievements have significant impacts on the development of Li-ion batteries.

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[4] Zhang, Y., and Faghri, A., 1996, "Heat Transfer Enhancement in Latent Heat Thermal Energy Storage System by Using the Internally Finned Tube," Int. J. Heat Mass Transfer, **39**(15), pp. 3165-3173.

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Scalable Routing and Broadcasting in Wireless ad hoc & Sensor Networks

by Amiya Nayak, Member EUAS

Short Biography

a) *NAME:*
NAYAK, Amiya, *Professor*
Member of Faculty of Graduate & Postgraduate Studies

b) *DEGREES:*
Ph.D., Systems & Computer Engineering, Carleton University, Ottawa, Ontario, 1991
M.C.S., Computer Science, Carleton University, Ottawa, Ontario, 1986
B.Math., Computer Science and Combinatorics & Optimization, University of Waterloo, 1982

c) *EMPLOYMENT HISTORY:*
2006 - *Professor, School of Information Technology & Engineering, University of Ottawa*
2002-06 *Associate Professor, School of Information Technology & Engineering, University of Ottawa*
1994-04 *Adjunct Research Professor, School of Computer Science, Carleton University*
1996-02 *Member of Scientific Staff, Nortel Networks, Ottawa*
1985-96 *Systems Designer, CMC Electronics, Ottawa*

d) *SCHOLARLY AND PROFESSIONAL ACTIVITIES (Since 2010):*
2018 - ***Associate Editor****, IEEE Internet of Things Journal.*
2017 ***Guest Editor****, IEEE Transaction on Industrial Informatics, Special Issue on Cloud Computing in Smart Grid Operation and Management.*
2016 ***General Co-Chair****, International Workshop on Security, Trust, Privacy and Analytics in conjunction with 30th IEEE International Conference on Advanced Information Networking and Applications (AINA-2016), Crans-Montana, Switzerland.*
2016 ***Steering Committee Member****, 2nd International Workshop on Future Information Security, Privacy and Forensics for Complex systems (FISP-2016) in conjunction with 11th International Conference on Future Networks and Communications (FNC-2016), Montreal.*
2016 ***Workshop Chair****, 13th International Conference on Mobile Systems and Pervasive Computing (MobiSPC'16), Montreal, Canada.*
2016 ***Steering Committee Member****, 1st International Workshop on Information Security and Privacy for Mobile Cloud Computing, Web and Internet of Things (ISCW-2016) in conjunction with 2016 IEEE International Conference on Cloud and Autonomic Computing (ICCAC), Augsburg, Germany.*
2015-- ***Editorial Board Member****, Journal of Sensor and Actuator Networks (JSAN), MDPI.*
2015-- ***Advisory Board Member****, International Journal of Distributed Sensor Networks (IJDSN), SAGE Publishing.*
2015 ***Publicity Chair****, Ad-Hoc, Mobile and Wireless Networks (ADHOC-NOW), Athens, Greece.*
2014 ***Workshop Chair****, 11th International Conference on Mobile Systems and Pervasive Computing (MobiSPC'14), Niagara Falls, Canada.*
2013 ***Technical Program Committee Chair****, 10th International Conference on Mobile and Ubiquitous Systems: Computing, Networking and Services, Tokyo, Japan.*
2013 ***Guest Editor****, IEEE Journal on Selected Areas in Communications, Special Issue on Networking Challenges in Cloud Computing Systems and Applications.*
2013 ***Technical Program Committee Chair****, IEEE WCNC Mobile Cloud Computing and Networking Workshop, Shanghai, China.*
2012 ***Program Vice-Chair****, 15th IEEE Int. Conference on Computational Science and Engineering, Nicosia, Cyprus.*
2012 ***Publicity Chair****, 4th FTRA Int. Conference on Computer Science and its Applications, Jeju Island, Korea.*
2011 ***Workshop Chair****, 13th IEEE Int. Conference on High Performance Computing and Communications (HPCC), Banff, Canada.*

2010 ***Program Vice-Chair****, 5th Int. Conference on Frontier of Computer Science & Technology (FCST), Changchun, China.*

2010- 2013 ***Associate Editor,*** *IEEE Transactions on Parallel & Distributed Systems.*

2008- 2015 ***Associate Editor****, EURASIP Journal on Wireless Communications & Networking, Hindawi Publishing Corporation.*

a) Scalable routing and broadcasting in wireless ad hoc and sensor networks

I have been working in this area for the past six years. My ongoing work in the field of wireless sensor networks (WSNs) has been mainly on the energy-conserving coordination and data communication in WSNs.

I have presented guidelines on how to design network layer protocols when the unit disk graph (UDG) model is replaced by a more realistic physical layer model. Instead of merely using the transmission radius in the UDG model, physical, MAC, and network layers share the information about a bit and/or packet reception probability as a function of distance between nodes. I have proposed a guideline for the design of greedy position-based routing protocols with known destination locations. The node currently holding the message forwards it to a neighbor (closer to the destination than itself) that minimizes the ratio of cost over progress, where the cost measure depends on the assumptions and metrics used, while the progress measures the difference in distances to the destination. This work was published in IEEE Communications Magazine, 43(3):101-106, 2005. This article serves as a preliminary contribution toward the development of network layer protocols that match the assumptions and criteria already used in simulators and ultimately in real equipment.

Applying the log normal shadow fading model to represent a realistic physical layer, I have proposed (i) a MAC layer protocol to produce the optimal shortest hop count routing scheme, (ii) a hop count optimal, greedy, localized routing algorithm, (iii) another algorithm called expected progress routing with acknowledgements, and (iv) a tR-greedy routing scheme, where the packet is forwarded to the neighbor closest to the destination, among neighbors that are within distance tR. These protocols were published in IEEE Journal on Selected Areas of Communications, 23(6):1267-1275, 2005.

We have investigated the problem of dynamic composition and management of virtual devices for ad hoc multimedia service delivery and proposed an autonomous policy driven framework for virtual device management. We have presented the framework components and methodology behind a policy-driven autonomous framework for the dynamic discovery, selection, and composition of multimodal multi-device services. We have also designed device/service discovery, composition, integration, and adaptation schemes for Mobile Ad hoc Network (MANET) environment, enabling users to generate, on-the-fly, complex strong specific systems, embedding in a distributed manner, QoS models providing compositions that form the best possible virtual device at the time of need.

We have investigated and proposed solutions for a wide range of problems (e.g., key distribution for secure communication, access control, routing, location service, area coverage, trust management) in mobile ad hoc networks and wireless sensor and robot networks. Moreover, I have co-authored a textbook, *Wireless Sensor and Actuator Networks: Algorithms and Protocols for Scalable Coordination and Data Communication*, published by John Wiley & Sons in 2010.

b) Fault tolerance & system-level fault diagnosis using evolutionary approaches

I have worked on a number of problems related to fault-tolerant computing, such as designing innovative mechanisms for recognizing catastrophic faults, applying the fundamental properties of the catastrophic faults to improve fault tolerance capabilities of networks, proposing new strategies for designing fault-tolerant peer-to-peer systems, and

system-level fault diagnosis using probabilistic genetic algorithms and other evolutionary methods. In the past, I have done complete characterization of catastrophic fault patterns for regular topologies. These are patterns of faults occurring in a system that can have catastrophic consequence regardless of the amount of built-in redundancies and reconfiguration capabilities. I have proposed efficient schemes for detecting, constructing and enumerating the catastrophic fault patterns, which can be used to assess reliability of a redundant system. This problem has practical importance because it deals with making a redundant system more reliable by choosing a proper interconnection structure to avoid catastrophic/cascading failure, taking advantage of the knowledge of fault patterns that arise in the field of application. This work will be used in the proposed research program to study fault propagation and the impact of communication networks on power grid and to design fault-tolerant topologies for preventing cascading failure.

I have considered various evolutionary approaches for system-level fault diagnosis. The problem of system-level fault diagnosis is computationally difficult and no efficient and generic deterministic solutions are known, motivating the use of heuristic algorithms. We have shown how artificial immune systems, ant colony optimization, swarm intelligence, neural networks, etc. can also be used for fault diagnosis in large multiprocessor systems containing several hundred nodes. As another major contribution in the area of fault tolerance, we have also a proposed a scheme to improve fault tolerance capabilities and search effectiveness in peer-to-peer systems. The proposed redundant strategy (Hybrid-Chord) improves the routing performance and data availability on Chord and De Bruijn topologies. The proposed scheme reduces the number of lookup hops significantly (by as much as 50%) compared to the original ones, and have better fault tolerance capabilities, with a small storage overhead. This work was published in IEEE Journal on Selected Areas in Communications, 25(1):6-15, 2007.

c) Characterization of Cascading Failure in Cyber Physical System & Smart Grid

I have investigated the cascading failure issue in interdependent cyber physical systems (CPS). We considered CPS as a system that consists of physical-resource and computational-resource networks, where these two are connected and mutually dependent. The failure in physical-resource network could cause the failures in computational-resource network, and vice versa. This failure may recursively occur and cause a sequence of failures in both networks. We proposed two novel models for the interdependent networks by using the complex network theory. Then, we studied the effect of cascading failures using percolation theory and presented the detailed mathematical analysis of failure propagation in the system. By calculating the size of functioning parts in both networks, we could analyze the robustness of our models in terms of the random attacks or failures. Our research proves that a tiny fraction of initial random failure could lead to the complete breakdown of the interdependent networks. The cascading failures in smart grid which is an example of CPS was also investigated, where two types of cascading failures are mixed. Contributions from these work have been published in top IEEE Transactions.

d) Distributed Access Control in Smart Grid and Cloud

As part of my recent research interests and activity in smart grids, I have been studying access control and fault tolerance issues for sometimes. We have proposed a decentralized security framework for smart grids that supports data aggregation and access control and a transport protocol for smart grids. It is important to secure the smart grid, not only from terrorist attacks, but also from customers and authorities who can tamper with various devices.

I have proposed a decentralized security framework for smart grids that supports data aggregation and access control. Data can be aggregated by home area network, building area network, and neighboring area network in such a way that the privacy of customers is protected. We used homomorphic encryption technique to achieve this. The consumer data that is collected is sent to the substations where it is monitored by remote terminal units (RTU). The proposed access control mechanism uses attribute-based encryption which gives selective access to consumer data stored in data repositories and used by different smart grid users. RTUs and users have attributes and cryptographic keys distributed by several key distribution centers (KDC). RTUs send data encrypted under a set of attributes. Since RTUs are maintained in the substations they are well protected in control rooms and are assumed to be trusted. Users can decrypt information provided they have valid attributes. The access control scheme is distributed in nature and does not rely on a single KDC to distribute the keys which makes the approach robust. To the best of our knowledge, ours is the first work on smart grids, which integrates these two important security components (privacy preserving data aggregation and access control) and the first paper which addresses access control in smart grids. We also proposed a new decentralized access control scheme for secure data storage in clouds that supports anonymous authentication. In the proposed scheme, the cloud verifies the authenticity of the series without knowing the user's identity before storing data. Our scheme also has the added feature of access control in which only valid users are able to decrypt the stored information. The scheme prevents replay attacks and supports creation, modification, and reading data stored in the cloud. We also addressed user revocation. Moreover, our authentication and access control scheme is decentralized and robust, unlike other access control schemes designed for clouds which are centralized. The communication, computation, and storage overheads are comparable to centralized approaches.

Challenges in Predicting Crack Growth in Structures Operating in Extreme Environments

by Ashok Saxena, Member EUAS

Short Biography

Dr. Ashok Saxena *is a* ***Distinguished Professor and Dean Emeritus*** *in the Department of Mechanical Engineering at the University of Arkansas where in the past he has served as the* ***Provost and Vice-Chancellor of Academic Affairs*** *(2015-2016) the* ***Dean of Engineering and the Raymond and Irma Giffels****' Chair (2003-2012), and the Billingsley Endowed Chair (2014-2015). He is also an Adjunct Professor in the School of Materials Science and Engineering at Georgia Institute of Technology in Atlanta, GA.*

Dr. Saxena previously held the position of ***Regents' Professor and Chair*** *(1993-2002) of the School of Materials Science and Engineering at the Georgia Institute of Technology in Atlanta and was a Fellow Scientist at the Westinghouse Research and Development Center in Pittsburgh. He also served as the Vice Chancellor of Galgotias University in India for a two-year period between 2012-2014.*

Dr. Saxena received his MS and PhD degrees from University of Cincinnati in 1972 and 1974, respectively in Materials Science and Metallurgical Engineering and his B. Tech degree from the Indian Institute of Technology, Kanpur in 1970 in Mechanical Engineering.

Dr. Saxena's area of research is mechanical behavior of materials focusing on linear and nonlinear fracture mechanics and fracture in materials at high temperatures under creep and creep-fatigue conditions. He is the recipient of numerous awards and recognitions in the field of fracture research that include the George Irwin Medal (1992) from ASTM, the ASTM Award of Merit and Fellow (1994), Fellow of ASM International (1996), Fellow of International Congress on Fracture (2009) and Georgia Tech Outstanding Research Author Award (1993). He is a recipient of the Wohler Fatigue Medal from the European Structural Integrity Society (ESIS, 2010) and is an elected Fellow of the European Academy of Sciences (2016) and the recipient of the Paul C. Paris Gold Medal from International Congress on Fracture (2017). He has authored/co-authored/edited eight books and over 250 research publications.

Challenges in Predicting Crack Growth in Structures Operating in Extreme Environments

Considerations involved in predicting crack growth behavior of components that operate in extreme environments can be daunting because of the complexities of the materials and loading conditions involved and a plethora of damage mechanisms that can potentially be present such as creep deformation and damage, environment assisted cracking, and their synergistic play. These considerations are summarized as follows:

- Transient and steady-state thermal stresses
- Hold times and static and cyclic stresses due to external loading in fracture critical locations
- Environmental effects
- Creep deformation (primary, secondary, tertiary creep) and rupture
- Creep-fatigue and environmental effects
- Varying material properties due to temperature gradients
- Varying material properties due to anisotropy or microstructural gradients such as in weldments
- Complex crack geometries and variable amplitude loading
- In-service degradation of material properties

In creep-brittle materials, where there is competition between the evolution of crack tip stress fields due to time-dependent deformation and due to environment enhanced crack growth under sustained and cyclic loading, there are no unifying concepts that are currently available to characterize crack growth. This is a major gap in technology that currently exists and prevents the use of time-dependent fracture mechanics approach to an important class of high temperature materials such as Ni base alloys, directionally solidified (DS) materials, and single crystal (SX) materials. This paper critically reviews the promising approaches, and the needs for filling this technology gap. Recommendations for future work are made.

Fatigue Crack Growth Behavior of High Strength Ferritic Steels in High Pressure Hydrogen

Safe and low-cost, high-pressure hydrogen storage systems are a critical need for refueling stations for fuel-cell powered vehicles, for back-up power in residential and office buildings, and for fork-lifts in warehouses. These systems are also essential for harnesing clean power for reducing greenhouse gas emissions by tapping vast amounts of energy available from wind and sun.
Safe design for storage of hydrogen must consider the propensity of hydrogen to accelerate fatigue crack growth rates in the materials used in this application. American Society for Mechanical Engineers (ASME) has developed codes for designing pressure vessels for storing hydrogen but these codes are conservative because of gaps in our ability to confidently model the degradation kinetics of

hydrogen embrittlement in these steels. There has been progress in our understanding of mechanisms of hydrogen embrittlement in the crack tip process zone but not sufficient to allow development of robust models for predicting crack growth rates and how they are affected by variables such as loading frequency, load ratios, hydrogen pressure, gaseous impurities, temperature, and material variability.

Since the load ratios vary considerably and vary with duty cycles experienced by vessels during service, there is need for models to interpolate fatigue crack growth data for load ratio, R, ranging from $-1 \leq R \leq 0.8$. Similarly, the loading frequency, ν, can range from a cycle every few seconds to a cycle every few hours. Since no reliable models are available to interpolate effects of load ratio and frequencies on the fatigue crack growth rates, conservative assumptions are necessary leading to expensive designs.

In this study, fatigue crack growth rates were measured in the liner material in 10 MPa gaseous hydrogen at various load ratios, R, in the range $-1 \leq R \leq 0.2$ to address the need of autofrettaged cylinders. The lower hydrogen pressure was used because no experimental capabilities for testing at 100 MPa were available anywhere for testing negative load ratios. The effects of loading frequency were investigated and these results were compared with results from literature for similar alloys tested in 103 MPa gaseous hydrogen at positive R values. The differences in crack growth rates between H_2 pressures of 10 to 103 MPa as well as the effects of frequency on the environment assisted crack growth rates were assessed using pooled data from this study and previous studies.

FCGR behavior in high pressure gaseous H_2 environment at negative load ratios, R, of -1.0 and -0.5 were found to be comparable to those at load ratios of 0.1 and 0.2; the effects of load ratio become stronger for $R > 0.2$. The effect of decreasing loading frequency, ν, on the FCGR behavior in H_2 gaseous environment is small for frequencies less than 1 Hz. FCGR behavior in gaseous H_2 increases with increasing gas pressure and the magnitude of this effect appears to be highest in going from air environment to 10 MPa H_2 pressure and appears to saturate at 45 MPa. The impact of these variables on the design life of H_2 storage vessels is explored in this paper. It is shown that autofrettage can be used very effectively to enhance the fatigue life of these vessels especially when the minimum pressures associated with the duty cycles are fall below 55 MPa from a maximum value of 90 MPa.

Characterization of Nonlinear Effects in the Behavior of Composite Materials

by Evgeny Lomakin, Member EUAS

Short Biography

Professor Evgeny Lomakin *educated in Russia at the Faculty of Mechanics and Mathematics of the Lomonosov Moscow State University. He is the Head of the Department of Theory of Plasticity, Faculty of Mechanics and Mathematics, Lomonosov Moscow State University, Moscow; the Director of "Research Laboratory of Mechanics of Advanced Structural and Functional Materials", Perm National Research Polytechnic University, Perm, Ural Region of Russia; the Principal Researcher of Institute for Mechanical Engineering of Russian Academy of Sciences and Moscow Aviation Institute.*

He is the Corresponding member of Russian Academy of Sciences and the Member of EU Academy of Sciences, Doctor of Sciences (Physics and Mathematics). He is the member of the Boards of Editors of International Journals "Archive of Applied Mechanics", "Acta Mechanica", "Mechanics of Solids", "Mechanics of Advanced Materials and Modern Processes" (Springer). He is the member of EUROMECH (the European Mechanics Society), the member of ESCM (the European Society for Composite Materials) and ESIS (the European Structural Integrity Society), the member of Russian National Committee on Theoretical and Applied Mechanics, the member of The Council of National Board of Russian Academy of Sciences on Mechanics of Solids, the member of The Board of Experts of Supreme Certifying Commission of Russian Federation (scientific degrees), the Chief of The Board of Experts of Russian Foundation for Basic Research in Mechanics. He is The Honorable Professor of Lomonosov Moscow State University and Perm National Research Polytechnic University.

His main scientific interests are the experimental and theoretical studies of elastic and plastic deformation of porous, cracked and other heterogeneous materials of variable properties, fracture mechanics of these materials, rock mechanics, mechanics of non-linear thermoviscohyperelastic materials, mechanics of composite materials.

Evgeny V. Lomakin
Constitutive models of mechanical behavior of media with stress state dependent material properties

In Altenbach H., Maugin A., Erofeev V. (Eds.) Mechanics of Generalized Continua. Advanced Structured Materials, 2011, Vol. **7**, Springer-Verlag Berlin Heidelberg, pp 339-350

The features of the behavior of heterogeneous materials were studied. The dependence of effective elastic properties of micro-heterogeneous materials on the loading conditions were analyzed and the corresponding mathematical methods for the description of the observed effects were proposed. The constitutive relations of the theory of elasticity for isotropic solids with stress state dependent deformation properties were considered. The possible approach to the formulation of the constitutive relations for the elastic anisotropic solids that elastic properties depend on the stress state type was considered, and the

corresponding constitutive relations are proposed. The method for the determination of material's functions on the base of experimental data was proposed, too. The quite satisfactory correspondence between the theoretical results and the experimental data was shown.

T.A. Beliakova, E.V. Lomakin, Yu.P. Zezin
Experimental studies of thermoviscohyperelastic behaviour of filled elastomers

In Hans Irschik, Michael Krommer, Alexander K. Belyaev (Eds.) Advanced Dynamics and Model-Based Control of Structures and Machines. 2011. Springer-Verlag Wien, pp 27-34

The viscohyperelastic properties of the hydrogenated nitril-butadien rubber containing the nano-size particles of technical carbon are studied. The stress-strain curves and the relaxation diagrams of the material under conditions both of tension and compression are presented. For the description of the viscohyperelastic behavior of filled elastomers, the constitutive equations are proposed. These equations represent the experimental values of stresses as the sum of two parts: hyperelastic part and viscoelastic one. The hyperelastic part is determined by the hyperelastic potential. The viscoelastic one is described by the nonlinear analogue of the equations of linear theory of viscoelasticity. The method for the determination of the parameters and the material functions is proposed. The comparisons of experimental data with the results of theoretical predictions are presented.

E.V. Lomakin, P.A. Mossakovsky, A.M. Bragov, A.K. Lomunov, M.E. Kolotnikov, M.S. Vakshtein, F.K. Antonov
Investigation of impact resistance of multilayered woven composite barrier impregnated with the shear thickening fluid

Archive of Applied Mechanics, 2011, Vol. 81, Issue 12, pp 2007-2020

All the commercial jet engines must satisfy the safety regulations. The construction of engine must not allow any rotor fragments and above all, the fan blades to perforate the case of engine that is incident to engine failure. Recently, the containment design is being developed that is based on a softwall concept, consisting of relatively thin metal shell with a composite winding cover. The commonly used winding is a multilayered woven Kevlar fabric of high energy absorbing characteristics. The results of experimental and computational studies of the STF and Kevlar + STF composites behaviors under dynamic loads that were carried out to develop the mathematical model of impact interaction are presented in this paper. To determine the STF dynamic properties, the experimental studies using the Split Hopkinson Pressure Bar (SHPB) method were carried out. Comparative analysis of energy-absorbing capabilities of different protective shells was performed on the base of mathematical model. Two series of dynamic tests by the SPHB method in rigid and soft casings were carried out to determine the dynamic bulk and shear properties of STF. A simplified mathematical model of the STF was formulated for the use in computer simulation of ballistic impact tests of multilayered composite protective shells (Kevlar +STF). The study confirmed the hypothesis about the possibility to describe STF behavior by a Newtonian fluid model in the characteristic range of strain rate. The parameters of shear viscosity and bulk compressibility of the model were defined. It was concluded that the role of the contact conditions between STF and Kevlar basis in the process of increasing the energy absorption capacity of Kevlar-STF barrier is significant. It should be

noted that the mechanism of contact interaction between STF and Kevlar basis can be described by viscous friction law, i.e. the STF behaves almost as a rigid body during the interactions with the solids, while it normally behaves as a fluid. It was shown that the effectiveness of the STF impregnation for improving the protective properties of barriers is largely due to the internal friction. It was established that the STF impregnation of protective shells with titanium framework not only increases the absorption capacity of Kevlar package, but also reduces the deflection of the metal base.

E. V. Lomakin, B. N. Fedulov, A. M. Melnikov
Constitutive models for anisotropic materials susceptible to loading conditions

In Hans Irschik, Michael Krommer, Alexander K. Belyaev (Eds.) Mechanics and Model-Based Control of Advanced Engineering Systems. © Springer-Verlag Wien 2014 Wien, 2014, pp 209–216

The mechanical behavior of many structural materials displays anisotropic elastic and plastic properties in different degree. Along with anisotropy, their behavior may demonstrate the asymmetry in the mechanical properties. The simplest example of this asymmetry is the difference of the deformation characteristics or the yield limits under conditions of tension and compression in the same directions in a material. Generally, the mechanical properties of materials may be expressed as the functions of direction of the applied load and some parameters of the stress state type. In some of recently proposed theories of elasticity and plasticity different from the classic isotropic theories based on the Hooke's law and Tresca or von Mises yield criteria, the anisotropy and asymmetry of the mechanical properties in some degree are involved, but the formulation of general equations that may be easily used in engineering is still a challenged problem. In this paper, generalized constitutive equations for the description of elastic and plastic behavior of anisotropic materials with stress state dependent properties are considered.

E.V. Lomakin, B.N. Fedulov
Nonlinear anisotropic elasticity for laminate composites

Meccanica, 2015, Vol. 50, Issue 6, pp. 1527-1535

Many structural materials, which are preferred for the developing of advanced constructions, are inhomogeneous ones. These materials have complex internal structure and properties, which make them to be more effectual in the solution of special problems required for development engineering. On the other hand, in consequence of this internal heterogeneity, they exhibit complex mechanical properties. In this work, the analysis of some features of the behavior of composite materials under different loading conditions is carried out. The dependence of nonlinear elastic response of composite materials on loading conditions is studied. Several approaches to model elastic nonlinearity such as different stiffness for particular type of loadings and nonlinear shear stress–strain relations are considered. Instead of a set of constant anisotropy coefficients, the anisotropy functions are introduced. Eventually, the combined constitutive relations are proposed to describe simultaneously two types of physical nonlinearities, one of which characterizes the nonlinearity of shear stress–strain dependency and another one determines the stress state susceptibility of material properties. The method for experimental determination of material's functions is proposed. Quite satisfactory correlation between the theoretical

dependencies and the results of experimental studies is demonstrated. The nonlinear models proposed in this research have a general form and they are suitable for any heterogeneous materials but mostly are directed to anisotropic laminate composites subjected to loadings under plane stress conditions.

E.V. Lomakin, M. P. Tretyakov
Fracture properties of graphite materials and analysis of crack growth under bending conditions

Meccanica, 2016, Volume 51, Issue 10, pp. 2353-2364

Graphite materials are widely used as structural materials for load-bearing applications in different branches of technique, so the studies of fracture properties of these materials are important. These heterogeneous materials are multiphase, polygranular and contain pores, micro-cracks and other defects of structure to considerable extent, which cannot be eliminated by supplementary treatment, such as high temperature pressing and impregnation with pitch, or some other methods. The elastic, strength and fracture toughness properties of structural graphite materials were investigated in this work. The theoretical analysis and the experimental studies of crack growth were carried out for the bending conditions. The stable crack growth is observed for the initial relative crack length $\omega_0 \geq 0.27$ and unstable, non-equilibrium, growth - for $\omega_0 < 0.27$. Under a crack's stable behavior, fracture toughness is determined during the process of crack growth, and the critical value of the stress intensity factor is approximately constant for such a heterogeneous material as graphite. The crack growth rate can also be determined during the test. Cases of unstable crack growth are analyzed for different loading conditions. It has been shown that in the cases of unstable crack growth under the conditions of quasi-static loading, the stored energy is spent not only on the formation of a new crack surface but on kinetic energy of a beam, too, and these parts of energy can be comparable. The same conclusion is referred to the tests on impact strength where noticeable part of energy is spent on kinetic energy of sample's parts but not only on the formation of new fracture surface. The variation of kinetic energy can be described by corresponding equation that is obtained in a general form and can be used for arbitrary conditions of hard loading where cross-beam displacement is controlled. The results of this analysis can be equally applied not only to quasi-brittle materials, such as graphite, but to elastoplastic ones, too, in the cases when the requirements of linear fracture mechanics are satisfied.

E. Lomakin, S. Alexandrov, Yeau-Ren Jeng
Stress and strain fields in rotating elastic/plastic annular discs

Archive of Applied Mechanics, January 2016, Volume 86, Issue 1, pp 235-244

The von Mises yield criterion was used in conjunction with its associated flow rule to provide the elastic/plastic stress and strain distributions within the rotating annular discs made of perfectly plastic material under plane stress conditions. The solution for strain rates was reduced to one nonlinear ordinary differential equation and two linear ordinary differential equations. These equations can be solved one by one. The strain solution requires a numerical technique to evaluate ordinary integrals. An example was presented to illustrate the general solution. The general method proposed can be readily extended to orthotropic and pressure-dependent yield criteria.

Evgeny Lomakin, Lev Rabinskiy. Valery Radchenko. Yury Solyaev. Sergey Zhavoronok, Arseniy Babaytsev

Analytical estimates of the contact zone area for a pressurized flat-oval cylindrical shell placed between two parallel rigid plates

Meccanica, 2018, Vol. 53, Issue 15, pp 3831-3838

The paper presents an analytical estimate for an area of contact for a thin-walled noncircular cylindrical shell placed between two parallel rigid plates with an initial gap and then pressurized hydrostatically up to the contact appearance. The Euler–Bernoulli beam was used to model the shell deformation under the plane strain assumption. Such a simplification allows one to obtain the simplest closed-form estimate for the contact zone area. The first approximation was obtained neglecting the deformation of the curvilinear segments of the flat oval shell cross section while the solution for the curved beam loaded by the homogeneous pressure was considered as a second approximation. The accuracy of the proposed analytical solutions as well as their usability in the preliminary design of thin-walled elements of various cooling systems was validated by the results of both numerical simulations and experimental tests.

New Contributions in Biochemistry

by Etana Padan, Member EUAS

Short Biography

CURRENT POSITION/ADDRESS *: Professor, Dept. of Biological Chemistry, The Alexander Silberman Inst. of Life Sciences, The Hebrew University of Jerusalem*

ACADEMIC TRAINING

1958-1963	*Received M.Sc. degree with honors, Major subject: Biochemistry. Minor subject: Physiology and Genetics.*
1963-1969	*Received Ph.D. degree, Ph.D. Thesis: Study of the Properties of Blue-Green Algal Viruses." Worked under the guidance of Prof. M. Shilo, Department of Microbiological Chemistry. Hebrew University Hadassah Medical School.*

PROFESSIONAL EXPERIENCE

1969	*Appointed Instructor in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.*
1970	*Appointed Research Fellow (Lecturer) in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.*
1972	*Research Fellow in the Department of Biochemistry, Weizmann Institute, Rechovot. (Post Doctorate with Prof. M. Avron and Prof. H. Rottenberg).*
1973	*Visiting Fellow in the Department of Zoology, Rand Afrikaans University, Johannesburg, Republic of South Africa.*
1974	*Appointed Senior Lecturer in the Department of Microbiological Chemistry, Hebrew University.*
1977	*Received tenure (Senior Lecturer).*
1978-1979	*Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.*
1979	*Appointed Associate Professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*
1980	*Appointed the head of the Oceanography programme in the Hebrew University.*
1982	*Appointed a science advisor in Biochemistry by the Binational Science Foundation.*
1983	*Member of the organizing committee of the 2nd International Workshop on primary productivity held in April, 1984, Haifa, Israel.*
1985	*Appointed full professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*
1985-1986	*Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.* *Member of the Editorial Board of FEMS Microbiology Reviews.*
1988	*Member of the organizing committee of the 6th International Symposium on Photosynthetic Prokaryotes, Holland, August, 1988.*
1989	*Head of Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*
1990	*Visiting Professor in the Department of Biochemistry, Mount Sinai Medical Center of the University of New York.*
1992-1995	*Head of Institute of Life Sciences, Hebrew University of Jerusalem, October, 1992.*
1995	*Awarded M. Launda Prize of the Israeli Payis Institute for "Understanding of Physiology of Microorganisms and Their Adaptations to Changing Environment."*
1996	*Awarded EMBO Fellowship, Visiting Professor with Prof. H.*

	Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.
1998	*Chairperson of The Second FISEB, Societie of Experimental Biology, Eilat December, 1998.*
1998-2001	*Prorector of the Hebrew University of Jerusalem.*
1999	*Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.*
2000-2006	*Editor for Biomembrane Section of Biochem. Biophys Acta*
2001	*Elected to the American Academy of Microbiology*
2002	*Member of the International Advisory Board of the XIII EBEC, European Bioenergetic Conference, Pisa 2004*
2004	*President-Elect of the Israeli Society of Biochemistry and Molecular Biology*
2004	*Advisory Board of E-MeP, The European Membrane Protein Consortium, 2004-2009.*
2005	*Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.*
2005	*Faculty 1000 Biology chosen paper.*
2006	*Member of Bikura panel. Israel Science Foundation.*
2009	*Editorial Advisory Panel Member of Molecular Membrane Biology.*
2011	*Member of the organizing committee of the EBEC, European Bioenergetics Conference*
2012	*Invited lecture in the EDICT symposium Portugal, Trevira*
2012	*Invited lecture in the meeting: The Intricate workings of membrane proteins, Jerusalem*
2013	*Invited lecture in the International Congress of Molecular and Cell Biology, July, Suzhou.*
2013	*Invited to deliver this years' Lars Ernster Lecture in Bioenergetics at the Department of Biochemistry and Biophysics at Stockholm University, Sweden.*
2014	*Invited Plenary-lecture in EBEC, European Bioenergetics Conference, Lisbon, July, 2014.*
2014	*Invited lecture at Membrane Transport and Communication,Riedberg, Germany.*
2015	*Invited lecture at the Antiporters Structure and Function meeting, Frankfurt, Germany.*
2015	*Chairperson, Annual Meeting of The Israel Society for Biochemistry and Molecular Biology, Focus on Membrane Proteins. November, Bar-Ilan University, Israel.*
2015	*Invited lecture at the Workshop on Structural and Functional Dynamics of Na+/H+ Antiporters, November, Frankfurt, Germany.*
2016	*Invited lecture at the Symposium in Memory of Prof Haim GartyRegulation of Sodium Transport in Health and Disease,January, Weitzmann Institute of Science.*
2016	*Invited lecture at the 80th Birthday of H.R. Kaback, NIH, Washington DC, USA*
2016	*Chairperson and organizing commeetee EBEC, European Bioenergetics Conference, Italy.*
2017	*Awarded the Ilanit- Katzir Prize for outstanding research achievements in the Life Sciences*
2017	*Elected member of the EU Academy of Sciences*
2018	*Awarded the Mitchell Prize and medal for outstanding research in bioenergetics and molecular and structural biology of NhaA, the Na+/H+ antiporter. 20th European Bioenergetics Conference (EBEC) Budapest, Hungary 25-30 August, 2018*

Asp133 Residue in NhaA Na^+/H^+ Antiporter Is Required for Stability Cation Binding and Transport

Abraham Rimon[1], Manish Dwivedi[1], Assaf Friedler[2] and Etana Padan[1]

1 - Department of Biological Chemistry, Alexander Silberman Institute of Life Sciences, Edmond J. Safra Campus, Givat Ram, Jerusalem 91904, Israel 2 - Institute of Chemistry, Faculty of Sciences, Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, Jerusalem 91904, Israel

J. Mol. Biol (2018) 430, 867-880.

Na+/H+ antiporters have a crucial role in pH and Na+ homeostasis in cells. The crystal structure of NhaA, the main antiporter of *Escherichia coli*, has provided general insights into antiporter mechanisms and revealed a previously unknown structural fold, which has since been identified in several secondary active transporters. This unique structural fold is very delicately electrostatically balanced. Asp133 and Lys 300 have been ascribed

essential roles in this balance and, more generally, in the structure and function of the antiporter (Figure 1).

In the present study, our aim was to identify the structural/functional roles of Asp133 in NhaA. To this end, we mutated Asp133 in CL(Cys less)-NhaA to several other amino acid residues(i.e.,Ala, Cys, Lys), varying in the polarity and length of their side chains, and we characterized how these mutations affected the antiporter's stability and function. In parallel, we used accessibility tests of sulfhydryl (SH) reagents to the Cys replacement D133C to study the conformation of D133C as a function of pH, in situ in cells treated with EDTA and in vitro in detergent micelles. These studies revealed that the mutants could still perform partial Na^+/H^+ antiport activity even when Asp133 was replaced with putatively neutral or positive residues. However, all mutants displayed lower thermal stability compared with wild-type (WT) NhaA, indicating the importance of Asp133 for optimal NhaA structural stability and function.

Remarkably, at alkaline pH, D133C both *in-situ* and *in-vitro* was shown to undergo a conformational change such that it was directed outward, enabling SH reagents of limited size to access and chemically modify D133. Notably, however, when D133C was exposed to [2-(trimethyl ammonium)ethyl] methanehiosulfonate bromide (MTSET), which chemically modified its side chain, the protein bound Li^+ with a Kd similar to that of WT NhaA, implying that the peptide bond of Asp133, rather than the residue's side chain, is what contributes to Li^+ binding. Taken together, the results reveal that Asp133 fulfills three roles in NhaA: it binds the ligand and, changes conformation with pH to open the periplasmic funnel, and is critical for NhaA stability.

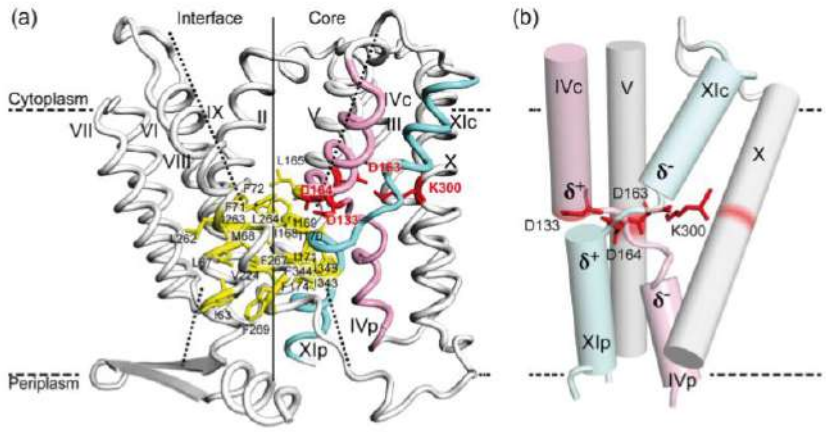

Fig. 1. Crystal structure of NhaA highlighting the TM IV/XI assembly and the hydrophobic barrier. (a) The crystal structure of NhaA (PDB entry 4 AU5) is viewed parallel to the membrane as a ribbon representation. The TMs are numbered by Roman numerals, and TMs I and XII are deleted for clarity. The NhaA fold, with topologically inverted TM IV and TM XI colored pink and light blue, respectively, is crossing each other where they are interrupted by an unwound portion (extended chains) that split them into cytoplasmic (c) and periplasmic (p) segments. The other TMs are colored grey. The funnels are indicated by dotted lines, and the membrane by broken lines. All highlighted amino acids are represented by sticks and colored either red (in the cation binding site) or yellow (in the hydrophobic barrier). (b) The non-canonical TM IV/XI assembly shown in cylindrical presentation. The partially negatively charged C-termini of the interrupted helices IVp and XIc and the partially positive dipoles of the N-termini of helices IVc and XIp oppose each other, and the charges are compensated by Lys300 and Asp133, respectively.

Replacement of Lys-300 with a glutamine in the NhaA Na^+/H^+ antiporter of *Escherichia coli* yields a functional electrogenic transporter

Miyer Patiño-Ruiz[1], Manish Dwivedi[2], Octavian Călinescu[3], Mehmet Karabel[1], Etana Padan[2], Klaus Fendler[1].

J. Biol. Chem. (2018) (In press)

From the 1 Max-Planck Institute of Biophysics, 60438 Frankfurt am Main, Germany; 2 Institute of Life Sciences, Hebrew University of Jerusalem, 91904 Jerusalem, Israel; 3 "Carol Davila" University of Medicine and Pharmacy, 050474 Bucharest, Romania

Much of the research on Na^+/H^+ exchange has been done in prokaryotic models, mainly on the NhaA Na^+/H^+ exchanger from *Escherichia coli* (EcNhaA). Two conserved aspartate residues, Asp-163 and Asp-164 (Figure 1), are essential for transport and are candidates for possible binding sites for the two H^+ that are exchanged for one Na^+ to make the overall transport process electrogenic. More recently, a proposed mechanism of transport for EcNhaA has suggested direct binding of one of the transported H^+ to the conserved Lys300 residue, a salt bridge partner of Asp-163 (Figure 1). This contention is supported by a study reporting that substitution of the equivalent residue, Lys-305, of a related Na^+/H^+ antiporter, NapA from *Thermus thermophilus*, renders the transporter electroneutral.
In this work, we sought to establish whether the Lys300 residue and its partner Asp-163 are essential for the electrogenicity of EcNhaA. To that end, we replaced Lys-300 with Gln, either alone or together with the simultaneous substitution of Asp-163 with Asn, and characterized these transporter variants in electrophysiological experiments combined with H^+ transport measurements and stability analysis. We found that K300Q EcNhaA can still support electrogenic Na^+/H^+ antiport in EcNhaA, but has reduced thermal stability. A parallel electrophysiological investigation of the K305Q variant of TtNapA revealed that it is also electrogenic. Furthermore, replacement of both salt bridge partners in the ion-binding site of EcNhaA produced an electrogenic variant (D163N-K300Q). Our findings indicate that alternative mechanisms sustain EcNhaA activity in the absence of canonical ion-binding residues and that the conserved lysines confer structural stability.

Broad phylogenetic analysis of cation/proton antiporters reveals transport determinants

Gal Masrati[1], Manish Dwivedi[2], Abraham Rimon[2], Yael Gluck-Margolin[2], Amit Kessel[1], Haim Ashkenazy[3], Itay Mayrose[4], Etana Padan[2] & Nir Ben-Tal [1]
Nature Communication (2018) 9: 4205- 4250.

From 1 Department of Biochemistry and Molecular Biology, George S. Wise Faculty of Life Sciences, Tel-Aviv University, Ramat-Aviv, 69978 Tel-Aviv, Israel; 2 Department of Biological Chemistry, The Alexander Silberman Inst. of Life Sciences, The Hebrew University of Jerusalem, Jerusalem 91904, Israel; 3 Department of Cell Research and Immunology, George S. Wise Faculty of Life Sciences, Tel-Aviv University, Ramat-Aviv, 69978 Tel-Aviv, Israel; 4 Department of Molecular Biology and Ecology of Plant, George S. Wise Faculty of Life Sciences, Tel-Aviv University, Ramat-Aviv, 69978 Tel-Aviv, Israel.

Cation/proton antiporters (CPAs) play a major role in maintaining living cells' homeostasis. CPAs are commonly divided into two main groups, CPA1 and CPA2, and are further characterized by two main phenotypes: ion selectivity and electrogenicity. However, tracing the evolutionary relationships of these transporters is challenging because of the high diversity within CPAs. Previous phylogenetic studies have mainly surveyed the evolutionary relationships between CPAs of limited diversity. These analyses divided CPAs into CPA1 and CPA2, which occasionally are stated to relate to the phenotypical electroneutral/ electrogenic partition. Specifically, the common idea is that CPA1s are electroneutral, while CPA2s are electrogenic. However, this partition has yet to be truly established, and there is still much debate concerning the mechanism behind electrogenicity, as the data are conflicting. Additionally, the exact molecular determinants that confer ion selectivity are still unclear.

Exploiting the recent flood of protein sequence, we study the evolutionary relationships among 6597 transporters that encompass the enormous richness of CPAs. We combined two newly developed bioinformatics methods for this analysis. The reconstructed phylogeny divided the CPA sequence pool into two groups, with high bootstrap values of 93%. By mapping proteins that are classified as CPA1 and CPA2 onto the tree, we conclude that the observed two groups reflect these two main CPA subtrees. Moreover, some distinct clades within the tree appear to consist of proteins that share electrogenic properties and/or are potassium selective. Thus, the phylogenic tree appears to reflect the main characteristics of the CPA superfamily. We reveal a well defined sequence motif (Figure 2) that distinguishes CPA1s from CPA2s and appears to determine the characteristics of electrogenicity and ion selectivity. Our findings imply that the phylogenetic division of the CPA superfamily only partially corresponds with the functional electroneutral/electrogenic partition, in contrast to previous suggestions. Finally, to experimentally test our computational analysis, we design a triple mutant that rescues an inactive EcNhaA variant, further supporting the importance of two acidic residues in the binding site to electrogenicity. Our analysis further indicates two acidic residues in the binding site that carry the protons in electrogenic CPAs, and a polar residue in the unwound transmembrane helix 4 that determines ion selectivity. A rationally designed triple mutant successfully converted the electrogenic CPA, EcNhaA, to be electroneutral.

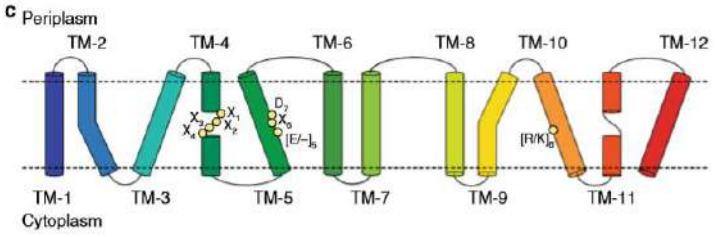

Fig. 2 The CPA motif is located in the core domain, near the ion binding site. Schematic two-dimensional representation of EcNhaA's structure. The membrane boundaries are shown as dashed lines, the helices are numbered TM-1through-TM-12, and the motif residues are indicated with yellow spheres

Diode Assisted Magnetoresistance in Semiconductors and Reconfigurable Spin Logic

by Xiaozhong Zhang, Member EUAS

Short Biography

Prof. Xiaozhong Zhang is Professor of School of Materials Science and Engineering, Tsinghua University (China), Professor of Beijing Innovation Center for Future Chip, China, and Professor of Center for Brian-Inspired Computing Research, Tsinghua University (China).

Prof. Zhang received B.Sc. in Physics from Fudan University (1982), M.Sc. in Condensed Matter Physics from Shanghai Jiaotong University (1984). In 1985 he won Chinese Government Scholarship to study PhD in Materials Science at University of Oxford (1985-1989) and received his D.Phil from University of Oxford (1989). He then worked as a postdoctoral research fellow at Royal Institution of Great Britain for three years. During 1992-1999 he worked as a research fellow, then lecturer and then senior lecturer at Department of Physics, National University of Singapore. In 1999 he came to Tsinghua University (China) to work as a Professor at Department of Materials Science and Engineering.

He was the director of Electron Microscopy Laboratory of Tsinghua University (1999-2006) and deputy director of central laboratory of Department of Materials Science and Engineering, Tsinghua University (1999-2006). He has been deputy director of the Education Ministry Key Laboratory of Advanced Materials (1999- present). He had been served as the deputy chief of Chinese national nano-technology standardization committee, member of consulting committee of Chinese analytic and measuring society and member of Chinese national micro-beam analysis standardization committee. He is now member of Chinese national nano-technology standardization committee and consultant member of Chinese national micro-beam analysis standardization committee.

His research interests are spintronic materials and devices, carbon materials, nanomaterials and nanostructure, superconducting materials, electron microscopy, and computational materials science. He has published more than 200 referred journal papers and been award 25 patents. He is now a co-editor of IUCrJ and editorial member of other four scientific journals. He received First Prize of Chinese Analytic and measuring society (2003). His course "Electron Microanalyses" was selected as a National Elite Course (2007). His silicon based magnetoresistance work was selected as "Top 10 University level scientific and technological advances of the year of 2011 in China" (2011) and "Top 10 scientific advances of the year of 2011 in China" (2011)

Diode-assisted geometry enhanced magnetoresistance in semiconductors

Non-ferromagnetic materials InSb, Bi, Ag2±δSe, Ag2±δTe and even Si have been reported to exhibit huge magnetoresistance (MR) at large field than their magnetic counterparts such as giant magnetoresistance (GMR) and tunneling magnetoresistance

(TMR) structures, which aroused broad interest for their potential impact on magnetic sensing industry. Unfortunately, normal MR of non-ferromagnetic semiconductor was limited by mobility and geometry. However, researchers reported in succession at room temperature extraordinary huge MR effects in silicon, all of which went beyond the limitation of normal MR. The field sensitivity of these MRs was even approaching that of GMR structures. These MRs in silicon, though resulting from different mechanisms, shared some common characteristics. The MR values were all positive and much larger than ordinary MR. The dependence of MR on magnetic field tended to be linear at large field. More interestingly, the abnormal MRs all occurred at nonlinear electro-transport regions.

We presented a diode assisted geometry enhanced MR (DAGEMR) device based on silicon [C.H. Wan et al, Nature, **477**, 304-307, (2011); Z.C Luo et al. JAP, **117**, 17A302, (2015)]. Lightly phosphorus-doped Si wafers were selected for fabricating MR devices. Indium electrodes were used to make contacts with wafers at four corners. Two voltage-stabilizing diodes were used to connect the current source and the voltmeter (Fig.1). The transport properties were all measured using four-terminal method at 300 K. Magnetic field of 1.2 T was applied perpendicularly to plane. The MR of this device is dependent with the geometry of the device, i.e. $MR \propto (W/L)^3$. At magnetic field of 1.2T, the MR was ~100% at W/L=20 and the MR was ~10000% at W/L=100. The abnormally enhanced MR named as diode-assisted geometry enhanced MR (DAGEMR) could be attributed to combination effect of Hall Effect of silicon and nonlinear effect of diode. The diodes provided a transition area where the MR could be enhanced dramatically. These MR devices based on the DAGEMR mechanism might build a bridge between microelectronics and magnetic sensor industry. We also applied this DAGEMR mechanism to other semiconductors, such as Ge and GaAs. The large MR of ~1000% was also realized. [J.M. Wang, et al, JAP **114**, 034501 (2013); J.J. Chen, et al, APL, **105**, 193508 (2014)].

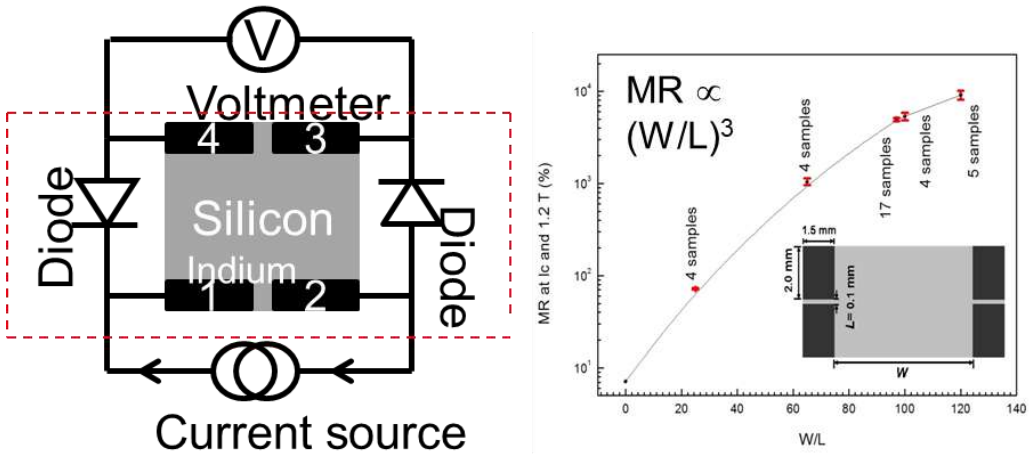

Fig.1 Schematic of diode-assisted MR device, and MR vs W/L.

We further applied this DAGEMR mechanism to magnetic material Ta/CoFeB/MgO which is PMA material [Z.C. Luo et al, Adv. Mater. **28**, 2760 (2016)]. The extremely large MR of 22000% was realized at 1mT. The abnormally enhanced MR in this magnetic

material could be attributed to combination effect of Anomalous Hall Effect of magnetic material and nonlinear effect of diode.

We further studied if the diode needed for generation such large MR. We fabricated two-terminal devices on silicon wafer that was moderately doped with phosphorous (n-type). The electron density and electron mobility were measured as 3×10^{15} cm^{-3} and 300 cm^2 V^{-1} s^{-1}, respectively. Then a heavily doped n-type region extending to ~1 μm below each electrode area with an electron density of 10^{18} cm^{-3} was formed by using phosphorous ion implantation. Subsequently, the electrode layers of titanium and aluminum were deposited for measurement. A large room temperature MR of >1000 % could be realized at small magnetic field of 0.05 T [ZC Luo， et al. Adv. Electron. Mater. **3,** 1700186 **(**2017)]. Its MR mechanism could be attributed to as following: In silicon which is associated with the impurity onsite Coulomb interaction and the space charge limited current (SCLC), delocalization of electrons in doubly occupied traps with a strong onsite Coulomb interaction leads to an S-shape negative differential conductance (SNDC) due to the presence of SCLC. A large MR will appear around the SNDC region.

Reconfigurable spin logic combined with non-volatile memory writing

Silicon-based complementary metal-oxide-semiconductor (CMOS) transistors have achieved great success. However, the traditional development pathway is approaching its fundamental limits. Magnetoelectronics logic, especially magnetic-field-based logic, shows promise for surpassing the development limits of CMOS logic and arouses profound attentions. Existing proposals of magnetic-field-based logic are based on exotic semiconductors and difficult for further technological implementation. We proposed a kind of diode-assisted geometry-enhanced low-magnetic-field MR mechanism. It couples p-n junction's nonlinear transport characteristic and Lorentz force by geometry, and shows extremely large low-magnetic-field MR (>120% at 0.15 T). Further, it is applied to experimentally demonstrate current-controlled reconfigurable magnetoresistance logic on the silicon platform at room temperature [ZC Luo et al. Adv. Func. Mater., **25,** 158, (2015)]. This magnetic logic device (Fig.2) could perform reconfigurable all four basic Boolean logic including AND, OR, NAND and NOR in one device. Combined with non-volatile magnetic memory, this logic architecture with unique magnetoelectric properties has the advantages of current-controlled reconfiguration, zero refresh consumption, instant-on performance and would bridge the processor-memory gap. Our findings would pave the way in silicon-based magnetoelectronics and offer a route to make a new kind of microprocessor with potential of high performance. The mechanism of magnetic logic used in silicon was applied to PMA material Ta/CoFeB/MgO. We realized non-volatile configurable all four basic Boolean logic including AND, OR, NAND and NOR in the device made by Ta/CoFeB/MgO [Z.C. Luo et al. Adv. Mater., **28**, 2760, (2016)].

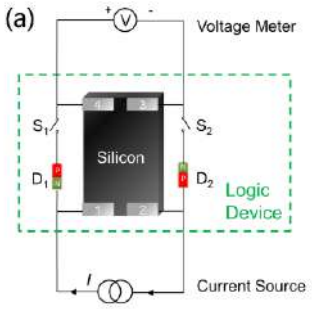

Fig.2. Schematic of magnetic logic device

We further proposed a novel spin logic based on PMA material Ta/CoFeB/MgO [Z.C. Luo et al. Adv. Mater., **29**, 1605027 (2017)]. By coupling anomalous Hall effect in magnetic materials and negative resistance effect in semiconductors, all four basic Boolean logic operations including AND, NAND, OR and NOR, can be programmed by a magnetic bit at room temperature with high output ratio ($>10^3$ %). In the same clock cycle of reconfigurable logic, benefit from built-in spin Hall effect in magnetic multilayer, logic results can be directly written into magnetic bits by all-electric method without dynamic magnetic field, demonstrating information reading, processing and writing realized in one step and one simple device. This logic-memory computation procedure offers a feasible platform to build a magnetic computer with potential of low dissipation and high performance.

Pioneering Activities in Research & Development that Influenced International Geotechnical Engineering

by Heinz Brandl, Member EUAS

Short Biography

Heinz Brandl was born on 29.06.1940 in Znaim/Lower Austria (now Znojmo, Czech Republic). He graduated 1963 in Civil Engineering with a Dipl.-Ing. (M.Sc.) from the Technical University in Vienna, from where he also obtained the degree of Dr.techn. (PhD) in Geotechnical Engineering with summa cum laude in 1966. From 1963 to 1966 he was Assistant at the Institute for Soil Mechanics and Ground Engineering at the Vienna Technical University, then Assistant Professor and Head of the Soil Mechanics Laboratory. In 1971 he was appointed Associate Professor (with Habilitation) but left the University to pursue comprehensive practice and applied research as a freelance consulting engineer for numerous projects and construction sites in Austria and abroad.

In 1977 H. Brandl was appointed Full Professor for Soil and Rock Mechanics and Foundation Engineering (including Tunnelling) at the Technical University of Graz. From 1978 to 1981 he was Head of the Geotechnical Institute in Graz, and since 1981 he has been Full Professor at the Technical University of Vienna chairing until 2009 the prestigious Institute for Soil Mechanics and Geotechnical Engineering, which was founded by Prof. Karl Terzaghi in 1928. Since 2008 he is Prof. Emeritus.

Professor Brandl's creative work comprises about 580 scientific publications (mostly as sole author, including 21 books), partly published in 18 languages. The subjects cover laboratory and field testing, soil and rock mechanics, foundation engineering, slope engineering, earthworks, tunnelling, urban undergrounds, restoration of historical buildings, road and railway engineering, hydro/hydraulic engineering and environmental engineering (landfills, waste deposits, brownfield remediation), geosynthetics, geothermal engineering ("energy foundations", "energy tunnels" etc.), natural disaster mitigation and rehabilitation, etc. He also published on philosophical aspects and on ethics in the profession (e.g. at the DFI Conference in Vienna, 1998; at the 1st International Conference on Geotechnical Engineering Education and Training, 2000 in Romania; then in Australia, Canada, Germany, Russia, USA, etc.).

From the very outset of his professional work H. Brandl has been bridging the gap between theory and practice. He has been fully responsible for nearly 4000 projects of civil engineering, geotechnical and environmental engineering in Austria and elsewhere: e.g. retaining structures up to 70 m height, high motorway embankments (up to 135 m in Austria and Greece), risky slope stabilizations, bridges in unstable terrain, all Danube Bridges in Austria since 1976, Beska Bridge in Serbia (2009) and other challenging river bridges, highways, high-speed railways and metros, deep soil improvements, high-rise structures (Highland Towers in Kuala Lumpur, Millennium Tower in Vienna, etc.), deep excavations, waste disposal facilities, contaminated land rehabilitation, dams, river renaturation, power plants, offshore structures, industrial buildings and buildings under difficult conditions (soft ground, seismic areas, areas of subsidence), flood protection, rockfall and avalanche protection, torrents' regulations, etc. In 2013 he was invited to develop a Master Plan for Sudan's Capital Khartoum.

By creating a semi-empirical design method and taking calculated risks (combined with contingency plans), he achieved not only significant cost savings but could also combine his engineering activities with many opportunities for comprehensive research work leading to numerous theoretical and practical innovations.

His innovations in geothermal geotechnics ("energy foundations" and other energy ground structures) are an important contribution to environmental protection. For instance, all new metro stations of Vienna are equipped with geothermal heating and cooling. Meanwhile this idea has spread worldwide for all kinds of buildings.

His experience comprises soil and rock investigations, general and detailed planning, design and calculation, construction work, engineering consulting, construction management and control, overall supervision, long-term monitoring and remedial works. This synergy between science and practice has significantly fostered basic research, innovations and applied sciences. Moreover, numerous students, scientists and assistants could thus be educated as persons with a wide professional spectrum.

Prof. Brandl has been active worldwide since 1968 as chairman, general reporter, state-of-the-art reporter,

special-, keynote- and opening lecturer, discussion leader and panellist at numerous international conferences on soil and rock mechanics, ground engineering, road and bridge engineering, environmental engineering, geosynthetics, etc. Up to now he delivered nearly 600 different invited lectures worldwide (also as visiting professor), covering the entire professional field.
Professor Brandl was First Vice-President of the International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE) for the period 1997-2001. From 1972 to 2015 he was President of the Austrian Society for Soil Mechanics and Geotechnical Engineering (now Honorary President). Furthermore, he has been chairman and board or core member of numerous national and international technical committees for geotechnical engineering, road and transportation research, waste management and land remediation, hydropower, flood protection, natural disaster mitigation and rehabilitation, geosynthetics, and preservation/restoration of old buildings, etc. since the Seventies. Since then he has also been a member of advisory boards, scientific committees and paper review committees of numerous international conferences worldwide, and a member of editorial boards and peer review committees of international scientific journals (presently 36 journals).
Until now his international activities have covered 104 countries on all continents.
In 1992 Professor Brandl was appointed foreign member of the Royal Academy of Sciences of Belgium, and since 1997 he has been member of the New York Academy of Sciences. He received numerous national and international awards, 19 honorary doctorates and other honours (e.g. Austrian Cross of Honour 1st Class for Sciences and Arts; Honorary Professor of Perm State Technical University, Russia).
He was the Rankine Lecturer of the year 2001 (London) and the Manuel Rocha Lecturer of the year 2008 (Lisbon). Moreover he was J. Mitchell Memorial Lecturer of the Deep Foundations Institute (DFI), USA 1998; the first K. Széchy Lecturer in Hungary (1994), the first E. Nonveiller Lecturer in Croatia (2000), the L. Suklje Lecturer in Slovenia (2003), etc., and he created the prestigious "Vienna Terzaghi Lecture". He was Millennium Lecturer (Joint World Conference of ISSMGE, ISRM, IAEG) in 2000, Melbourne; the Giroud Lecturer at the World Conference of IGS (International Geosynthetics Society) in 2010, Brazil; the 10th Distinguished CW Lovell Lecturer (Jubilee Event) at Purdue University, USA, 2011; the E. de Beer Memorial Lecturer, Belgium; the 75th Anniversary of ISSMGE Lecturer, Athens 2011; the H. Lorenz Lecturer, Germany, 2013; the 50th Anniversary DECGE Lecturer 2014.
Since June 2003 Prof. Brandl has been President of the Austrian Society of Engineers and Architects, which was founded already in 1848 and has been the "umbrella" organisation of Austria's Engineers and Architects since.

Prof. Brandl's pioneering activities in research and development that influenced international geotechnical engineering

- Development of the worldwide first research room to investigate the freezing-thawing behaviour of soils and other granular materials (1963). Air temperature between +25° C and -40° C, simulation of ground water, precipitation and growth of ice lenses. Comprehensive test series led to important criteria for road and railway engineering already in the late 1960s and early 1970s.

- Comprehensive basic research on the shear strength of soils and weathered rock, especially regarding residual strength and progressive failure, since the 1960s.

- Comprehensive investigation of grain crushing and fine particle increase during compaction of granular materials, and its influence on freezing-thawing behaviour and bearing capacity of road structures in the late 1960s and early 1970s; leading to detailed guidelines for practice.

- Soil stabilization with lime, cement and other additives in the 1960s and 1970s. Laboratory and field tests led to international guidelines and codes.

- Comprehensive research in pavement geotechnics (road and highway engineering) between the late 1960s and 1980s – leading to detailed guidelines, also for rail tracks (design, execution, control), considering not only geotechnical aspects but also

economical, environmental, lifecycle, sustainability, serviceability and maintenance aspects. Fundamentals for high-speed railway engineering.

- Development of retaining structures consisting of small diameter piles (root piles etc.) as composite systems considering the pile-soil interaction in vertical and horizontal direction ("bar walls") – mainly for underpinning of buildings during undercrossing or adjacent excavations (Metros, etc.) in the late 1960s to 1970s.
- Comprehensive research on long-term settlements (creeping) of soils since 1970.
- Comprehensive theoretical research and field measurements of special cases of lateral earth pressure: earth pressure redistribution, compaction pressure, and especially creeping pressure (in unstable slopes) since the early 1970s; leading to relevant design and calculation methods.
- Development of the "semi-empirical design method with calculated risk" in geotechnical engineering (also using the "observational method"); in the early 1970s. This led to significant cost savings during the past decades.
- Soil and rock nailing from the early 1970s to the 1980s.
- Innovative methods of underpinning, re-tilting and re-levelling of existing buildings in the 1970s and 1980s.
- Deep box-shaped foundations (e.g. "pile-boxes", piled rafts) of high-rise buildings, river bridges, bridges in sliding slopes, for seismic zones, etc. since the 1970s.
- Geosynthetics since 1970 in research and practice of civil engineering (and architecture), especially in geotechnical, hydro, road and railway engineering.
- Deep soil improvement with heavy tamping, deep dynamic consolidation and deep soil-lime mixing ("lime piles") since the early 1970s.
- Advanced earthwork since the 1970s. Highway embankments up to 135 m height on heterogeneous ground or along unstable slopes (fill materials from silt to rock).
- Special foundations and protection of large bridges along sliding/creeping slopes (e.g. caissons up to 27 m diameter and 45 m depth). Comprehensive research in connection with design, risk analyses, calculation, execution and (long-term) monitoring since the 1970s.
- Flexible and rigid culverts (up to 10 m diameter) in or below high embankments; earth pressure distribution, design and construction in the 1970s and 1980s.
- Long prestressed ground anchors (up to 150 m length) in research and practice, especially in the 1970s and 1980s; then spreading worldwide.
- Multiple anchored retaining structures of different systems (continuous walls, spaced panel walls, beams, ribs, etc.) up to 60 m height in unstable slopes, along deep slope cuts, in excavation pits; in the 1970s and 1980s.
- Research, development, design and construction of crib walls ("green walls") up to 45 m height and along unstable slopes, especially in the 1970s and 1980s.

- Comprehensive research on pile diameters (d = 0,1 to 6 m) and geometry of pile foundations regarding skin friction and group effects in the 1970s and 1980s.
- Caisson walls ("pier walls") of intermittent reinforced concrete caissons (up to 9 m diameter and 60 m depth) with different shaft sinking methods; in the early 1980s.
- Chemical grouting – comprehensive comparative investigations (laboratory tests, field tests, site measurements) and environmental aspects (e.g. long-term influence on groundwater) in the 1980s.
- Development and optimization of engineered landfills, mainly municipal and hazardous waste deposits since the early 1980s (e.g. multi-barrier systems).
- Development of the cellular double-wall vertical barrier system for municipal and hazardous waste containment and for groundwater management along dykes and levees in urban areas; early 1980s to the 1990s.
- Comprehensive research and practice in the field of contaminated ground (brownfield) restoration and renaturation since the late 1980s.
- Piled embankments on soft soils and peat: since 1970s for highways; since 1990 for high- speed railways (stone columns, piles and composite fill structures).
- Roller-integrated continuous compaction control (CCC) since the late 1980s and especially in the 1990s – leading to international guidelines and standards in road and railway engineering, for dams and dykes, for landfills, etc.
- High-speed railway engineering, considering the entire system of interacting structural elements from subsoil to the rail-wheel-subsystem (1990 – 2005).
- Near-surface geothermal engineering since the late 1980s. Promotion of "energy foundations", "energy tunnels", etc. for heating and/or cooling all sorts of buildings
- Comprehensive research and practice in the field of flood protection. Optimization of flood protection dams, dykes and levees, especially since the year 2000 (based on earlier own scientific activities between 1965 and 1995).

Thermodynamics & Kinetics of Nanomaterials

by Qing Jiang, Member EUAS

Short Biography

Qing Jiang is Professor of the School of Materials Science and Engineering, Jilin University, and Director of the Key Laboratory of Automobile Materials, Ministry of Education, China. He received his BSc and MSc in Materials Science from Jilin University of Technology (combined into Jilin University in 2000) in 1982 and 1984, respectively, and PhD in Chemistry from University of Stuttgart, Germany in 1990. After working at Technical University of Berlin as a postdoc for two years, Dr. Jiang joined Jilin University of Technology as a professor in 1992. In 2000, he was granted The National Science Fund for Distinguished Young Scholar by National Natural Science Foundation of China. In 2001, Dr. Jiang was awarded as the Chueng Kong Scholar Professor from Ministry of Education, China. During the time from 1996 to 2012, Dr. Jiang worked as vice dean/excusive vice dean of school of Materials Science and Engineering, Jilin University. As visiting professors, Dr. Jiang worked in University of California (Irvine), USA (1997), Forschungszentrum Karlsruhe, Germany (1999), and Tohoku University, Japan (2013).

Now Dr. Jiang is a Fellow of The Institute of Physics (U.K.), an Academician of the Asia Pacific Academy of Materials and a Member of the EU Academy of Sciences. He also serves several international journals as the members of the editorial board or advisory boards. He earned the first class prize of science and technology of Jilin province, China, for two times.

Dr. Jiang has published more than 500 papers in peer-reviewed journals, including Nature series, Cell series, Adv. Mater., Phys. Rev. Lett., Angew. Chem. Int. Ed., Environ. Energy Sci., et al, which have been cited more than 15,000 times with h-index of 64 (Web of Science). Contributions have also been recorded in 1 monograph, 16 monographic reports and over 50 keynote or invited talks at international conferences. In addition, Dr. Jiang has supervised/co-supervised more than 60 PhD students.

Research

Thermodynamics is a phenomenological theory that can predict stable phase structure and surface properties of macroscopic materials under a certain ambient conditions, and plays a key role in design of novel materials for a wide range of technologies. However, owing to neglecting significant surface effect of nanomaterials with ultrahigh surface/volume ratio, this theory is generally unreliable, or even invalid. Therefore, one of central issues in materials science is to develop thermodynamic methodology for correctly illustrating and exactly predicting the physicochemical properties of nanomaterials and then propose proper design of high-performance materials.

The research objective is to establish intrinsic relationships between basic thermodynamic functions and size and shape of materials, extend thermodynamics to

nanoscale to predict stable phase and surface properties of nanomaterials, and design and develop multifunctional nanomaterials for high-performance and -efficiency applications. The principal scientific achievements are listed as follows:

(1) Developing thermodynamics of nanomaterials to discover intrinsic relationship between internal energy and size of nanomaterials and establish surface energy functions of nanomaterials. These discoveries provide thermodynamic basis to regulate surface energy and adsorption energy of nanomaterials in many important applications.

Based on the Lindemann melting criterion, we established an analytic $T_m(D)$ function without any free parameter:

$$T_m(D)/T_m(\infty) = \exp\{[-2S_{vib}(\infty)/3R]/(D/D_0-1)]\}$$

where ∞ denotes the bulk size, $S_{vib}(\infty)$ is the vibrational entropy, $D_0 = 2(3-d)h$ with d being the dimension and h being the atomic or molecular diameter, and R is the ideal gas constant. While further achieving size-dependent function of melting entropy $[S_m(D)]$ according to Mott′s theory on $S_{vib}(\infty)$, size-dependent melting enthalpy $H_m(D)$ was given by $H_m(D) = T_m(D)S_m(D)$. In light of the similar physical natures of melting and evaporation phenomena, we further developed the size-dependent internal energy $E_c(D)$:

$$E_c(D)/E_c(\infty) = \exp[(-2S_{eb}/3R)/(D/D_0 - 1)][1 - 1/(D/D_0 - 1)]$$

wherein $S_{eb} = E_{eb}/T_{eb}$ with S_{eb}, E_{eb} and T_{eb} being evaporation entropy, evaporation enthalpy and evaporation temperature for bulk materials, respectively, and $D_0 = h/2$.

Considering that both interface energy and interface stress are two important thermodynamic parameters to determine the atomic structures of interfaces and dominate the regulation of advanced functional properties of nanomaterials, we proposed their quantitative expressions at the interfaces among solid, liquid and gas states according to the internal energy difference between interfacial and interior atoms:

$$\gamma(D)/\gamma(\infty) = [1 - 1/(2D/h - 1)] \exp[(-2S_{eb}/3R)/(2D/h - 1)].$$

Here a modified bond-breaking model was proposed to propose a surface energy function of bulk materials:

$$\gamma(\infty) = [(2 - m - \sqrt{m}) + \beta(2 - n - \sqrt{n})E_c(\infty)]/[(2 + 2\beta)N_a A_s]$$

with $m = Z_s/Z_b$ (Z_s and Z_b are coordination numbers of surface and interior atoms), N_a denoting the Avogadro constant, A_S being the unit area of two dimensional cell, $n = Z'_s/Z'_b$ (Z'_s and Z'_b denote the second-nearest coordination numbers of surface and internal atoms) and β the ratio of the sum of second-nearest bond strength to that of the nearest bond strength. These thermodynamic functions of nanomaterials not only extend the application of thermodynamics into nanometer scale to illustrate the physical essence of size effect of physicochemical properties, but also offer quantitative database to precisely describe surface properties.

(2). Following the theoretical prediction according to thermodynamics of nanomaterials, we proposed coupling methodologies of materials selection, size/crystallographic structure

control to maximize adsorption energy of nanomaterials, and discovered synergistic mechanisms of size, alloying, strain, and interface effects to achieve moderate adsorption energy. Following these principles, we developed high-adsorption-capacity nanomaterials for trace-molecule detection and moderate-adsorption-energy catalysts for high-efficiency catalysis.

High-performance sensing materials generally rely on the high-surface-energy materials to realize strong adsorption via selecting materials with high surface energy and decreasing their sizes to nanoscale in addition to strain engineering that effectively improves the adsorption energy. By making use of these synergistic methodologies, we developed various advanced adsorbent nanomaterials and exploring their applications for CO trace-molecule detection. A principle of the enhancement of CO adsorption was developed through doping single-atom Al into graphene. After CO adsorption, evident electron transfer from Al to CO triggers a semiconductor-to-conductor transition in Al-incorporated graphene systems. Therein, the band gap of Al-incorporated graphene recovers to zero. As a result, the Al-incorporated graphene exhibits outstanding sensitivity for ppb CO detection.

Catalytic reactions require catalysts to have a proper adsorption energy that ensures the kinetic balance between adsorption of reactant molecule/intermediate and desorption of reactant product for realizing the optimization of reaction rate with high selectivity and resistance to poisoning. Unary metallic Pd usually exhibits exceptionally low catalytic activity towards formic acid dehydrogenation reaction due to its high surface energy/adsorption energy. To reduce the adsorption energy, low surface energy element of Au and small atomic radius element of Co were introduced into the Pd structure to make a CoAuPd alloy. Co in the internal core generates compressive stress at the surface and at the same time, there occurs electrons transfer from Pd to Au due to the lower electronegativity of Pd, resulting in the decreases of the surface energy of surface Pd atoms, leading to the enhanced catalytic activity. To further achieve a moderate adsorption energy, metal/support interface was fabricated by growing PdNi nanoparticles on NH_2-functionalized N-doped graphene. The strong interaction between the substrate and NiPd nanoparticles which leads to electron transfer from support to Pd and the alloying of Pd with Ni can reduce the surface energy of Pd atoms. Therefore, the PdNi/NH_2-functionalized-N-doped graphene exhibits remarkably enhanced catalytic activity for formic acid dehydrogenation.

(3). According to theoretical predictions of thermodynamics of nanomaterials, we discovered the relationships between electrode structure and electron and ion transport kinetics, following which we designed and developed three-dimensional nanoporous electrodes for high-performance electrochemical biosensor and energy storage devices.

High-performance electrochemical biosensors require the electrode to have not only high-adsorption-energy materials but also high electron transfer and sufficient available surface. To satisfy these requirements, we proposed a facile strategy to develop monolithic hybrid electrodes with minimized electrical resistivity. By the combination of in-situ electrochemical alloying/dealloying and hydrothermal methods, we developed nanoporous Au/Co_3O_4 hybrid microelectrodes which exhibit ultrahigh sensitivity, fast response, high reliability and selectivity in glucose detection.

Electrochemical capacitor can deliver high levels of electrical power and offer long lifetimes, but their energy storage density is too low for many important applications. To address the challenge in realizing high-density energy storage at fast charge/discharge rates, we proposed that phase transformation of metallic vanadium sesquioxide could yield high-ordered oxygen vacancies to enhance the cation accessibility, extending two-dimensional (surface) to three-dimensional (bulk) storage. We further developed symmetric wind voltage window pseudocapacitors, which deliver a power density of carbon-based supercapacitor together with an exceptionally high volumetric energy density, being much higher than lithium thin-film batteries.

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Research Activities within the Energy Group

by Mohsen Assadi, Member EUAS

Short Biography

Present positions

- Professor, Gas technology, Univ. of Stavanger, Norway, since 2007.
- Head of energy efficiency research group at Univ. of Stavanger, Norway, since 2015.
- Visiting professor at Sheffield University, UK, 2016-2018.

Previous position

- *Professor in Thermal Power Engineering, Dept. of Energy Sciences, Lund University, Sweden (2006-2011).*
- *Chief Scientist, Ineternational Research Institute of Stavanger, Norway, 2008-2015.*
- *Director, Center for Sustainable Energy Sloutions (cenSE), Norway, since 2009-2015.*
- *Visiting professor at Leeds University, UK, 2009-2014*

Education

- *PhD in Thermal Power Engineering, Dept. of Energy Sciences, Lund University, Sweden.*
- *MSc in Mechanical Engineering, Lund University, Sweden.*

Courses and education

I had the main responsibility for undergraduate and master level courses as well as PhD courses at division of Thermal Power Engineering at Lund University and at University of Stavanger.

Course leader and curriculum design for under graduate courses at Stavanger University and Lund University

Theory of Turbomachinary
Applied Thermodynamics
Steam and Gas Turbine Technology
Project course in Energy Conversion Technology
Energy and environment
From gas to electricity
Drilling and well construction

PhD Courses

- *Thermal Design and Optimization*
- *Theory of Turbomachinery*
- *Physical and Chemical Equilibrium*
- *Seminars in Power Plant Technology*
- *Artificial Neural Network for plant monitoring*

Main fields of competence

Mohsen Assadi's research activities are focused on environmental friendly energy technologies, comprising energy system integration, carbon capture and storage (CCS), energy conversion technologies, e.g. gas turbines, fuel cells and steam cycles utilising various fossil and renewable energy sources; system modelling, integration, optimization and monitoring, data driven modeling based on Artificial Neural Networks (ANN).

Project leadership

Mohsen Assadi has been project leader for several nationally financed project in Sweden and

Norway as well as several EU-projects.
List of selected projects:

- *Energy system in transition (Marie Curie training program)*
- *Sustainable Energy Solutions (SIU-INCP)*
- *Roadmap for decarbonisation of Indian Energy system (SIU-INCP)*
- *Theoretical and experimental investigation of biogas fuelled technologies using advanced and intelligent modelling and monitoring tools (Bio-CHP-Monitor, NFR).*
- *Energy Efficiency Improvement via Waste Heat Recovery and Enhancement of Production Rate in Aluminum Industry (NFR).*
- *GAS-FACT, innovative carbon capture technologies for gas fueld power plants (Bilateral project).*
- *Low Emission Combustion Technology for Hydrogen-rich Syngas (H2-IGCC, EU FP7). Subproject leader for system integration.*
- *EU-GGC Clean Energy Network. EU-side working group leader for Clean Natural Gas Applications (EU, FP7).*
- *European North Sea Energy Alliance (ENSEA), holistic energy system integration for the North Sea region comprising environmental, technical, economic and political aspects (EU-FP7).*

Scientific leadership
Mohsen Assadi has been supervisor of 16 PhD students, which finished their studies with PhD degree and he is supervising 4 PhD students and 3 Post-Docs. Prof Assadi has been member of PhD defense committees of 17 PhD students at different European universities. He is also member of several advisory groups, associations and networks.

Research activities within the energy group at University of Stavanger, led by Prof. Assadi

Energy system in transition is the dominating topic of the energy research today. The complexity of the task is due to its multi-disciplinary nature, covering not only energy technology but also economy, policy, education and competence buildup as well as the environmental aspects of it.

The energy group at Department of Energy and Petroleum Engineering (IEP), at University of Stavanger (UiS), has been involved in a couple of projects and networks, aiming at addressing various aspects of the energy system in transition. This document provides a brief overview of some of the ongoing activities.

One of the main concerns of the energy industry today is availability of competent human resources trained to tackle the problems and challenges of the energy system of tomorrow. Therefore, education and training of the new generation of energy engineers need to be modified to fit the needs and requirements of the integrated energy system of tomorrow. Besides education and training of new generation of engineers, one also needs to deal with training of the existing work force. Smart technologies, smart meters, smart grid, digitalization, use of artificial intelligence and information communication technology (ICT) for monitoring and optimization of the energy system covering energy generation, distribution and consumption are among the topics that energy engineers have to deal with. Currently ongoing projects at IEP are specifically targeting training and knowledge buildup needed to support energy system in transition. One of the new initiatives at UiS has been establishment of a program area for geothermal energy that is aiming at facilitating multi-disciplinary research and knowledge transfer from the strong oil and gas sector to geothermal energy.

Projects

An EU-project, ENSYSTA (Energy Systems in Transition) funded by EU Horizon 2020 program under Marie Skłodowska-Curie grant agreement, finances 15 PhD students in six different

countries, i.e. Nederland, Germany, Scotland, Denmark, Sweden and Norway. This project aims at addressing energy system in transition from a multi-disciplinary point of view. The North Sea region was selected as living lab for the project, due to its potential concerning combination of renewable energy such as wind and wave energy, and petroleum resources and infrastructure. Energy system modeling, using open source approach was selected as the main focus area. The multi-level and multi-dimension modeling tools to be developed will enable analysis of various future scenarios that will provide better decision support for future investments in the North Sea region. The outcome of this project will support fulfillment of the ambitious goals of the EU concerning CO2 reduction and implementation of clean energy system by 2050. Various work packages in the project are supporting different aspects of the energy transition, namely system integration, energy technology, market and economy, as well as policy and environment. Using open source modeling will provide full access to the codes so that other research groups can adopt the models and tools developed or also further develop them towards their own specific goals and targets. https://ensystra.eu/

Two collaborative projects between India and Norway have been running in parallel, one ending in December 2018 and the other one in December 2019. These projects were aiming at knowledge and experience exchange within the field of clean energy between the two countries. Training of the workforce and development of curricula for energy education have been the main focus of these projects. One of the most fruitful activities have been organization of workshops in collaboration with the representatives of the energy industry to enable discussion and exchange of viewpoints between industry and academy concerning the content of the education and training programs, in order to insure that the needs of the energy industry are considered when developing new educational programs. Also a chapter book in two volumes and several scientific papers were published, addressing opportunities and challenges of the energy transition from both local and global point of view.

Program area for geothermal energy

Geothermal energy is considered as an important renewable energy source. However, its potential has not been fully developed yet, mainly due to high initial investment costs. Unlike wind and solar, geothermal energy is not an intermittent source of energy and the plants utilizing geothermal heat sources can be placed within densely populated areas. Such a placement would lead to reduced heat losses caused by transport over long distances. Geothermal energy can benefit from knowledge transfer from oil and gas sector. Knowledge domains such as geology, reservoir flow modeling, drilling and well construction which are central for oil and gas are also the core areas of competence needed for development of geothermal energy. To enhance knowledge transfer and cross-fertilization between the two fields of research, a program area for geothermal energy was established at University of Stavanger in 2018, led by Prof. Assadi.

University of Stavanger is well known for its petroleum research and has contributed substantially to development of Norwegian petroleum industry during the past decades. The program area for geothermal energy, combining the strong sub-surface expertise with a strong energy conversion and distribution, includes also researchers from other fields such as economy, social and political science, material technology, etc. This initiative, which is part of the UiS strategy towards clean energy, aims at facilitating multi-disciplinary R&D activities to support research and strengthen commercialization of the geothermal applications.

Smart sensors

Smart technologies and digitalization of the energy system requires access to operational data. Availability of accurate and affordable sensors is a key factor. However, calibration of advanced sensors is a time consuming and costly procedure.

The energy group at UiS has been actively utilizing artificial intelligence, specifically Artificial Neural Networks (ANN), for plant monitoring and control since late 1999. Within a collaborative research, together with Aachen University a successful effort was made to develop and evaluate advanced smart sensors, capable of self-calibration and data communication utilizing the existing

ICT infrastructure. The results of ANN modeling was compared to standard approaches and the results showed that same level of accuracy could be achieved. The ANN tool will be implemented in the sensor and automatic calibration and data communication will be tested in near future. The results of the study was presented in a scientific paper that is under review process for publication.

Innovative cycles

Energy efficiency has been highlighted as the most cost effective measure for emission reduction and thereby the most important contributor to combat the global warming. High efficiency in combination with enhanced CO2 capture capability, utilizing innovative solutions, was studied within collaborative research with UK and Belgium universities.

Experimental data and validated thermodynamic models were used to study characteristics of a small-scale solar plant with micro gas turbine (MGT). Operational optimization and techno-economic evaluation of the dish-based thermal solar with MGT was studied in detail and the results were published in a scientific paper.

The effects of exhaust gas recirculation in humid air turbines have been studied experimentally and theoretically both from technical and economic point of view. Results of the study have been published in a scientific paper.

Selected publication:

Books

1. "Sustainable Energy Technology and Policies, A Transformational Journey", Springer, Volume 1, ISBN 978-981-10-7187-4, ISSN 1865-3529, 2017, Editors: S. De, S. Bandyopadhyay, M. Assadi, D. A. Mukherjee.
2. "Sustainable Energy Technology and Policies, A Transformational Journey", Springer, Volume 2, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018, Editors: S. De, S. Bandyopadhyay, M. Assadi, D. A. Mukherjee.

Book chapters

1. A. Safari, S. Jafari, M. Assadi, "Role of Gas-Fuelled Solutions in Support of Future Sustainable Energy World"; Part I: Stimuluses, Enablers, and Barriers", Sustainable Energy Technology and Policies, A Transformational Journey Springer, **Volume 2**, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018.
2. A. Safari, N. Das, S. Jafari, O. Langhelle, J. Roy, M. Assadi, "Role of Gas-Fuelled Solutions in Support of Future Sustainable Energy World: Part II: Case Studies", Sustainable Energy Technology and Policies, A Transformational Journey Springer, Springer, **Volume 2**, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018.
3. H. Nikpey S., M. Assadi, "Micro-Scale Combined Heat and Power: Contributor to Sustainable Energy Solution", Sustainable Energy Technology and Policies, A Transformational Journey Springer, **Volume 2**, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018.
4. K. Parham, M. Assadi, "A Parametric Performance Analysis of a Novel Geothermal Based Cogeneration System", Sustainable Energy Technology and Policies, A Transformational Journey Springer, **Volume 2**, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018.
5. Assadi M., Mollayi Y., ""Dynamic Modeling of ORC Power Plants", Organic Rankine Cycle Technology for Heat Recovery, ISBEN number: 978-1-78984-348-4, 2018.

Journal publications

1. R. Avishek, J. Kuntal, M. Assadi, S. De, "Distributed polygeneration using local resources for an Indian village: multiobjective optimization using metaheuristic algorithm", Clean Technologies and Environmental Policy, 2018, 20:1323-1341, ISSN: 1618-954X, Springer.
2. M. Kamali, K. Parham, M. Assadi, "Performance analysis of a single stage absorption heat transformer based desalination system employing a new working pair of (EMIM) (DMP)/ H2O", International Journal of Energy Research, Volume 42, issue 15, pp. 4790-4804, DOI: 10.1002/er.4235, 2018.
3. Y. Mollaei Barzi, M. Assadi, K. Parham, "A waste heat recovery system development and analysis using ORC for the energy efficiency improvement in aluminium electrolysis cells", International Journal of Energy Research, DOI: 10.1002/er.3940, Nov. 2017.

4. A. Safari, H. Nikpey, K. Haji H., M. Assadi, "Application of an Experimentally Validated High-dimensional Surrogate Model to Performance Prediction of a CHP Unit", Energy Procedia 142 (2017) 1106–1111.
5. Majoumerd, M.M., Rass, H., Jana, K., De, S., Assadi, M. (2017): 'Coal quality effects on the performance of an IGCC power plant with CO2 capture in India', Energy Procedia (Elsevier) 114, 6478 - 6489.
6. U. Ali, C. Font-Palma, H. Nikpey, M. Mansouri, M. Akram, K. Finney, T. Best, N. Mohd Said, M. Assadi, M. Pourkashanian, "Benchmarking of a micro gasturbine model integrated with post-combustion CO2 capture", Energy 126 (2017) 475-487,http://dx.doi.org/10.1016/j.energy.2017.03.040.
7. Jana, K., Roy, A., Majoumerd, M.M., Assadi, M., De, S. (2017): Polygeneration as a future sustainable energy solution - A comprehensive review, Applied Energy (Elsevier), 202, 88-111.
8. Mondal, S., De, S. and Assadi, M. (2017): Waste heat recovery from flue gas containing SO2 through CO2 based combined power and refrigeration cycle, Journal of Energy and Environmental Sustainability, 3, 51-55.
9. Jana, K., Ray, A., De, S. Assadi, M. and Mondal, S. (2017): Performance of a biomass based polygeneration : Second law analysis, Journal of Energy and Environmental Sustainability, 3, 37-42.
10. Y. M. Barzi, M. Assadi, "Evaluation of a Thermosyphon Heat Pipe Operation and Application in a Waste Heat Recovery System", Experimental Heat Transfer, DOI 10.1080/08916152.2014.913089, pp. 493-510, Volume 28, Issue 5, 2015.
11. Mansouri Majoumerd, M., Nikpey H., Assadi M., Breuhaus P., "Micro gas turbine configurations with carbon capture - Performance assessment using a validated thermodynamic model", Applied thermal engineering [1359-4311], 2014 Volume:73, book:1, pp:170 -182.
12. Mansouri Majoumerd, M., Assadi M. "Techno-economic assessment of fossil fuel power plants with CO2 capture – Results of EU H2-IGCC project", International journal of hydrogen energy, Volum:39 Issue:30, pp. 16771 -16784, 2014.
13. Nikpey H., Assadi M., Breuhaus P., Mørkved P. T., "Experimental evaluation and ANN modeling of a recuperative micro gas turbine burning mixtures of natural gas and biogas", Applied Energy 2014; 117 (2014) 30–41.
14. Nikpey H., Mansouri M., Breuhaus P., Assadi M., "Performance analysis of a biogas-fueled micro gas turbine using a validated thermodynamic model", Applied Thermal Engineering 2014; 66 (2014) 181-190.
15. Mansouri Majoumerd M., Raas H., De S., Assadi M., "Estimation of performance variation of future generation IGCC with coal quality and gasification process – Simulation results of EU H2-IGCC project", Applied Energy 113 (2014) 452–462

Conference papers

1. De Paepe, Ward; Nikpey Somehsaraei, Homam; Giorgetti, Simone; Carrero, Marina Montero; Mansouri Majoumerd, Mohammad; Bram, Svend; Assadi, Mohsen; Laurent, Bricteux; Parente, Alessandro; Contino, Francesco. "Towards highly-flexible carbon-clean power production using gas turbines: exhaust gas recirculation and cycle humidification". The Future of Gas Turbine Technology, 9th International Gas Turbine Conference; 2018.
2. H. Nikpey Somehsaraei, U. Ali, C. Fonte-Palma, M. Mansouri Majoumerd, M. Akram, M. Pourkashanian, M. Assadi, "Evaluation of a Micro Gas Turbine with Post-Combustion CO2 Capture for Exhaust Gas Recirculation Potential with Two Experimentally Validated Models", GT2017-63551, Proceedings of ASME Turbo Expo 2017; Turbomachinery Technical Conference and Exposition, GT2017, June 26-30, 2017, Charlotte, NC, USA.

General Airgap Field Modulation Theory for Electrical Machines

by Ming Cheng, Member EUAS

Short Biography

Education

Ph.D. 2001 Department of Electrical & Electronic Engineering, The University of Hong Kong, Hong Kong

M. Phil. 1987 Department of Electrical Engineering, Southeast University (Formerly Nanjing Institute of Technology), China

B. Eng 1982 Department of Power Engineering, Nanjing Institute of Technology, China

Employment

2017-present Chair Professor, School of Electrical Engineering, Southeast University (SEU)
2015-2016 Distinguished Professor, School of Electrical Engineering, SEU
2000-present Full Professor, School of Electrical Engineering, SEU
1993-2000 Associate Professor, School of Electrical Engineering, SEU
1987-1992 Lecturer, School of Electrical Engineering, SEU

Honors/Awards

2018 Albert Nelson Marquis Lifetime Achievement Award
2018 China Industry-University-Research Cooperation Innovation Award
2018 Jiangsu Patent Inventor Award, China
2018 Silver Medal at the International Exhibition of Inventions Geneva
2016 Special Government Allowances of the State Council
2016 The Second Prize of National Technology Invention Award, China
2015 The First Prize of China Machinery Industry Science and Technology Award
2014 IET Premium Award in Electric Power Application
2014 Silver Medal at the International Exhibition of Inventions Geneva
2013 The First Prize of the Natural Science Award of the Ministry of Education of China
2013 Delta Scholar
2010 Award for Excellent Textbooks in Electric Power Industry
2010 Outstanding Workers of China Electrotechnical Society
2009 IET Achievement Award in Electric Power Application
2007 GM Automotive Innovative Talent Award for China University
2007 Jiangsu Provincial College Excellent Textbook Award
2006 SAE Environmental Excellence in Transportation Award
2005 The Second Prize of Jiangsu Science and Technology Progress Award
2004 Outstanding Scientific and Technological Workers in Jiangsu Province, China
1995 The Second Prize of Science and Technology Progress Award of State Education Com., China

Academic Qualifications

2008 Fellow of IET
2015 Fellow of IEEE
2015-2016 Distinguished Lecturer, IEEE Industry Application Society
2017 Member of the Administrative Committee (AdCom), IEEE Magnetics Society
2017-2018 Member-at-Large, IEEE Industry Application Society Executive Committee
2016-2019 Visiting Professorial Fellow in Aston University, UK

Editorial Board Positions

- *Editorial Advisory Board Member of "Energy Conversion and Management"*
- *Editorial Board Member of "Sustainable Energy"*
- *Editorial Advisory Board Member of "IEEJ Journal of Industry Applications"*
- *Editorial Board Director of "Journal of Electrical Engineering"*
- *Editorial Board Member of "Proceedings of CSEE"*
- *Editorial Board Member of "Transactions of China Electrotechnical Society"*
- *Editorial Board Member of CES Transactions on Electrical Machines and Systems"*
- *Co-Editor-in-Chief of Chinese Journal of Electrical Engineering.*

Publications

Authored/co-authored over 400 technical journal papers, over 200 international conference papers, 4 books and 4 book chapters. The 10 selected papers are as follows:

1. *Cheng Ming, Han Peng, Hua Wei. General airgap field modulation theory for electrical machines. IEEE Transactions on Industrial Electronics, August 2017, 64(8): 6063-6074.*
2. *Cheng Ming, Wen Honghui, Han Peng. Analysis of airgap field modulation principle of simple salient poles. IEEE Transactions on Industrial Electronics, April 2019, 66(4): 2628-2638.*
3. *Cheng Ming, Luo Rensong, Wei Xinchi. Design and analysis of current control methods for brushless doubly-fed induction machines. IEEE Transactions on Industrial Electronics, Jan. 2019, 66(1): 717-727.*
4. *Cheng Ming, Wang Jingxia, Zhu Sa and Wang Wei. Loss calculation and thermal analysis for nine-phase flux switching permanent magnet machine. IEEE Transactions on Energy Conversion, Dec. 2018, 33(4): 2133-2142.*
5. *Cheng Ming, Jiang Yunlei, Han Peng and Wang Qingsong. Unbalanced and low-order harmonic voltage mitigation of stand-alone dual-stator brushless doubly-fed induction wind generator. IEEE Transactions on Industrial Electronics, Nov. 2018, 65(11): 9135-9146.*
6. *Cheng Ming, Han Peng, Buja Giuseppe, and Jovanović G. Milutin. Emerging multi-port electrical machines and systems: past developments, current challenges and future prospects (Invited paper). IEEE Transactions on Industrial Electronics, July 2018, 65(7): 5422-5435.*
7. *Cheng Ming, Zhu Sa. Calculation of PM eddy current loss in IPM machine under PWM VSI supply with combined 2D FE and analytical method. IEEE Transactions on Magnetics, Jan. 2017, 53(1): Artile # 6300112.*
8. *Cheng Ming, Yu Feng, Chau K.T., and Hua Wei. Dynamic performance evaluation of a nine-phase flux-switching permanent magnet motor drive with model predictive control. IEEE Transactions on Industrial Electronics, July 2016, 63(7): 4539-4549.*
9. *Cheng Ming, Zhu Ying. The state of the art of wind energy conversion systems and technologies: A review (Invited Paper). Energy Conversion and Management, Dec. 2014, 88: 332-347.*
10. *Cheng Ming, Hua Wei, Zhang Jianzhong and Zhao Wenxiang. Overview of stator-permanent magnet brushless machines. IEEE Transactions on Industrial Electronics, November 2011, 58(11): 5087-5101.*

Electrical machines are physical devices to accomplish continuous electromechanical energy conversion through magnetic field coupling. Since Jacobi invented the first direct current machine (DCM) in 1834 and Ferraris and Tesla invented the first induction machine (IM) in late 1880s, electromagnetic machine has been a prime source of mechanical/electrical power for the past centuries. Besides the conventional DCM, IM and synchronous machine (SM), a vast variety of other electromagnetic machines have been resurging or emerging to meet various performance requirements, such as the permanent magnet brushless (PMBL) machines, the vernier machine, the brushless doubly-fed machine (BDFM), the stator-PM machines with doubly salient structure, the magnetic gear (MG) and magnetically-geared machine (MGM), and so on. Meanwhile, different analytical theories have been developed to analyze the underlying operation principle and electromagnetic performance of these machines, such as the winding function theory, the rotating field theory, two-reaction theory, the general theory based on the two-axis

primitive machine model and the general theory using equivalent magnetic circuits. Though all these established theories have ever brought great conveniences to analysis and design of conventional machines like DCM, IM, SM, etc., they show weakness in effectively analyzing a large proportion of newly-emerged machines with multi-harmonic and multi-port features, like BDFM, and stator-PM machines, etc. For example, the general theory developed by Adkins et al. based on the ideal machine model is only valid or accurate for AC machines with sinusoidal current, but not valid for DC machines.

With the unprecedented invasion of new electrical machine structures in the rush to electrification of the world during past decades, the theories and methods for analysis of operation mechanism, performance calculation and design principle, etc., are becoming more and more machine-specific and fragmented. Therefore it becomes a significant and urgent task to construct a systematic and theoretical explanation and guidance to invent, analyze and design new machine topologies to avoid blindness, contingency and overreliance on empirical knowledge.

An electrical machine usually has an airgap, which is a narrow layer of air, sandwiched by the stator, and rotor. Both the stator and rotor are made of soft magnetic materials featuring large relative permeance to air. PMs or field windings mounted on stator or rotor are to establish magnetic field whilst armature windings mounted on stator or rotor are to induce electromotive force (EMF) through cutting the magnetic lines.

As an electromechanical energy converter, the electrical machine shows remarkable resemblance to the switching converter, as illustrated in Fig. 1. Corresponding spectrums are also given to show the similarities in frequency domain.

According to the analogy, an electrical machine is a cascade of three elementary parts, that is, the primitive magnetizing magnetomotive force (MMF) (source), the short-circuited coil/variable reluctance/flux guide (modulator) and the armature winding (filter). The primitive magnetizing MMF establishes an initial MMF distribution with possible spatial harmonics along the physical airgap. The short-circuited coil/variable reluctance/flux guide modulates the initial MMF distribution to produce a spectrum of MMF harmonic components, for which they are termed as modulators. All the MMF components produce corresponding magnetic field components in the airgap. The armature winding plays the role of a spatial filter selecting effective airgap field harmonics to produce flux linkage or EMF, then feeds the electric load in generating mode or receives the synchronous current to provide mechanical output in motoring mode. The MMF component that can produce effective airgap field harmonic is termed as effective MMF component. The modulator is characterized by the modulation operator, which defines the mapping from primitive MMF distribution function to eventual MMF distribution function.

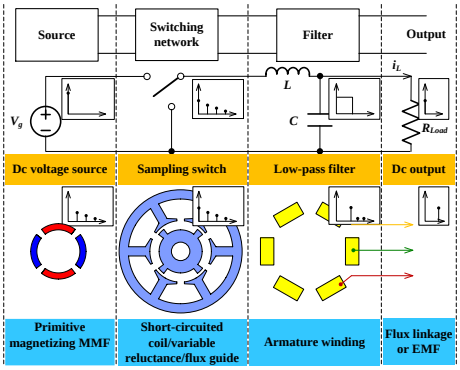

Fig. 1 Analogy between the electrical machine and the switching converter

By introducing the modulation operator, the physical airgap with windings, slots or flux guides nearby will be turned into an equivalent uniform one, as shown in Fig. 2, with the modulated MMF $M\left[F_f(\theta,t)\right]$ and $M\left[F_a(\theta,t)\right]$ expressed as:

$$M\left[F_{f(a)}(\theta,t)\right]=M_n\left[\cdots M_2\left[M_1\left[F_{f(a)}(\theta,t)\right]\right]\right] \tag{1}$$

where $F_f(\theta,t)$ is the primitive magnetizing MMF, $F_a(\theta,t)$ is the primitive armature MMF. And the airgap flux density distribution can be obtained as:

$$B_g(\theta,t)=\frac{\mu_0}{g}\left\{M\left[F_f(\theta,t)\right]+M\left[F_a(\theta,t)\right]\right\} \tag{2}$$

where B_g is airgap flux density, and μ_0 is the vacuum permeability. The electromagnetic torque can be derived as:

$$T_{em}(t)=-\frac{\mu_0 r_g^2 L_{stk}}{2g}\frac{\partial}{\partial\varphi}\int_0^{2\pi}\left\{M\left[F_f(\theta,t)\right]+M\left[F_a(\theta,t)\right]\right\}^2 d\theta \tag{3}$$

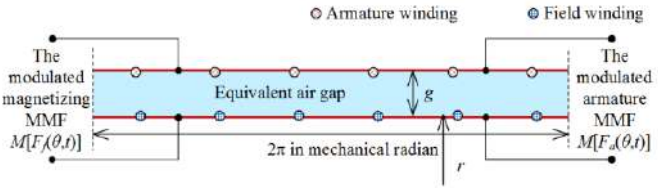

Fig. 2 The equivalent airgap model

Based on the proposed general field modulation theory, all electrical machines with magnetically anisotropic stator and rotor can be equivalent to a cylindrical one with an equivalent smooth airgap. General equations for no-load and loaded airgap field distributions, no-load flux linkage linked by armature winding, no-load EMF, and electromagnetic torque can be derived.

The superiority of the developed general airgap field modulation theory over existing ones can be summarized as:

1) It is valid for all electromagnetic machines, irrespective of DC or AC machines, salient or non-salient machines, sinusoidal or rectangular driving machines, etc.

2) It can perform not only the qualitative analysis with clear physical meaning, but also quantitative analysis of electrical machines.

3) It can not only analyze the available electric machines, but also guide the invention of new machine topologies.

Preformed Particle Gels: A Cost-effective and Efficient Solution to Control Water Production from Mature Oilfields and Improve CO2 Storage Efficiency

by Baojun Bai, Member EUAS

Short Biography

Education and Training

- *2006 Postdoc Fellow, Chemistry & Chemical Engineering Department, California Institute of Technology (Caltech), Pasadena, CA*
- *2005 Ph.D., Petroleum Engineering, New Mexico Institute of Mining and Technology, Socorro, NM, USA*
- *2002 Ph.D., Petroleum Geology, China University of Geoscience, Beijing, China.*
- *1995 MS., Petroleum Engineering, Graduate School of Research Institute of Petroleum Exploration and Development (RIPED), Beijing, China*
- *1992 BS., Reservoir Engineering, Northeast Petroleum University of China (Formerly, Daqing Petroleum Institute), Heilongjiang, China*

Academic Experience

- *Sept 2015-present, Professor, Lester Birbeck Endowed Chair, Petroleum Engineering Program, Department of Geosciences, Geological Engineering and Petroleum Engineering, Missouri University of Science and Technology (Missouri S&T, Formerly University of Missouri-Rolla, UMR), Rolla, Missouri, USA.*
- *Sept 2011-August 2015, Associate Professor, Lester Birbeck Endowed Chair, Petroleum Engineering Program, Department of Geosciences, Geological Engineering and Petroleum Engineering, Missouri S&T, Rolla, Missouri, USA.*
- *Aug 2006-Aug 2011, Assistant professor, Petroleum Engineering Program, Department of Geological Sciences and Engineering, Missouri S&T, Rolla, Missouri, USA.*
- *June 2005–July 2006, Postdoc Fellow, Division of Chemistry and Chemical Engineering, California Institute of Technology (Caltech), Pasadena, Ca, USA.*
- *May 2002–June 2005, Research Assistant (PhD student), New Mexico Petroleum Recovery Research Center (NMPRRC), Socorro, New Mexico, USA.*
- *Sept 1 1992–June 1995, Research Assistant (Master student), RIPED, China National Petroleum Corporation (CNPC), Beijing, China.*

Industry Experience

- *May – Aug 2007, Visiting scholar, Energy Technology Company, Chevron, Houston, TX, USA*
- *June 2005 – May 2006, Consultant, ChemEOR Inc, Covina, California, USA.*
- *June 1999 – May 2002, Director /Registered Petroleum Engineer, Conformance Control Laboratory, Research Institute of Petroleum Exploration and Development (RIPED), PetroChina Company Limited (PetroChina, formerly CNPC), Beijing, China.*
- *July 1995 – June 1999, Petroleum Engineer, Conformance Control Laboratory, RIPED, CNPC, Beijing, China.*

Major Awards and Honors

- *Member of EU Academy of Sciences, Elected in 2018*
- *Society of Petroleum Engineers (SPE) Mid-Continent Regional Service Award, 2018*
- *Changjiang Visiting Scholar/Professor, Ministry of Education, China, 2017*
- *SPE Mid-Continent Regional Distinguished Achievement Award for Petroleum Engineering Faculty, 2016*
- *Outstanding Teaching Award, 2014, 2015, 2017, Missouri S&T.*
- *Longjiang Visiting Scholar, 2012-2015, Heilong Jiang Province, P. R. China*
- *Lester Birbeck Endowed Chair in Missouri S&T, Since 2011*
- *Mines and Metallurgy Academy Faculty Award, Missouri S&T, April 2010*
- *Top Ten Best Achievements Award for Science and Technology Innovation, CNPC, 2005*
- *Golden Award for Science and Technology Innovation, CNPC and PetroChina, 2004*
- *Golden Award for Science and Technology Innovation, PetroChina, 2004*
- *Golden Award for Science and Technology Development and Innovation, RIPED, CNPC, 2001*
- *Winner of Top Ten Best Science and Technology Innovation Award, RIPED, CNPC, 2000*
- *Silver Award for Science and Technology Innovation and Transfer, CNPC, 1999*
- *Novel Low-cost Oilfield Development Technology Award, PetroChina, 1999*
- *Winner of Top Ten Best Science and Technology Innovation Award, RIPED, 1999*
- *Golden Award for Technology Innovation, RIPED,CNPC, 1998*
- *Silver Award of Science and Technology Development and Innovation, RIPED, CNPC,1998*
- *Top Ten Best Young Researchers, RIPED, CNPC, 1998*
- *Silver Award for Science and Technology Transfer, CNPC, 1997*
- *Excellent Employee Award, RIPED, CNPC, 1997*
- *Excellent Employee Award, RIPED, CNPC, 1996*
- *Silver Award for Science and Technology Innovation, RIPED, PetroChina, 1995*

Highlighted Scholarship Contributions

- **Preformed Particle Gels (PPG) for Conformance Control**: Gel treatment is an approved cost-effective method to reduce excess water production and improve oil recovery. Traditionally, in-situ gels were widely used for the purpose. In 1996, Dr Bai's research group first proposed to use preformed particle gels to control the preferential flow of water through channels and high permeability streaks because PPG was synthesized in surface facilities and can overcome some distinct drawbacks inherent in in-situ bulk gelation system such as lack of gelation time control, uncertainness of gelling due to shear degradation, chromatographic fractionation or change of gelant compositions, and dilution by formation water. Since then, his group has developed a series of particle gels with the size range of a few nanometers to millimeters and have carried out extensive experimental study to understand the transport behavior of particle gels through conduits, fractures, fracture-like channels, and porous media. He has recognized to be the pioneer in the particle gel conformance control area, which is evidenced by the follows:
  - He was awarded multiple projects regarding to particle gel conformance control by PetroChina/CNPC, US DOE, major oil companies, and service companies. The projects mainly focus on new product development and their applications in harsh reservoirs conditions, understand the mechanisms of particle gel propagation and blocking in different high permeable features and provide a new tool to optimize PPG treatment design to benefit oil production, from which people can identify where and how particle gel technology could be best used.
  - It is estimated that the technology has been applied in nearly 10,000 wells worldwide, mostly in China.
  - His research group has published more than 100 papers related to PPG technology in peer reviewed journals and proceedings of prestigious national/international petroleum conferences.
  - His research group (Led by Yifu Long, Jiaming Geng and Xindi Sun) has successfully

developed a series of CO_2 stimulated/sensitive nano- to milli-meter (mm) sized novel polymer particles (Figure 1) to improve the sweep efficiency and storage efficiency of CO_2 storage in mature oilfields.

- His research group (Led by Jingyang Pu) has successfully developed re-crosslinkable preformed particles gels (Figure 2) that can be used to control the fluid flow in abnormal features in mature reservoirs, such as wormholes, Matrix Bypass Event (MBE), Caves, and so on.
- His research group (Led by Ze Wang and Xindi Sun) has proposed a major mechanism that polymer gel block fractures and has done extensive lab tests to approve it (Figure 3), which is of major importance to improving the design of gel treatments in fractures.
- His research group (Led by Jiaming Wang) investigated the EOR mechanism of Nanogels (Figure 4) and found that the nanogels were able to spontaneously reduce oil-water interfacial tension and stabilize oil/water emulsion by forming adsorbed layer at the oil-water interface. In addition, it has been found that nanogels can adsorb onto rock surface and modify wettability driven by electrostatic interaction and the Wan der Waals' force. The rock surface turned to become water-wet after nanogel adsorption due to the hydrophilic properties of nanogels. From the core flooding experiments, he found nanogels can fragment large oil drops (spontaneous emulsification) and increase the residual oil recovery and divert chasing fluid in microscopic level. Nanogels can decrease the relative permeability of water while not affect the relative permeability of oil.

(a) Nanogel swelling (b) mm-sized PPG (before swelling) (c) mm-sized PPG after

Fig. 1. Series of Particle Gel Products

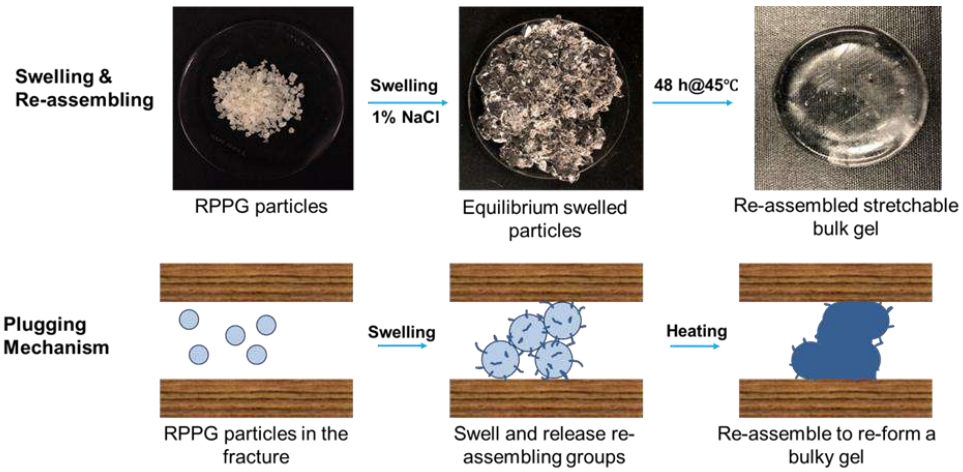

Fig. 2. Re-crosslinkable Preformed Particle Gel and Plugging Mechanism

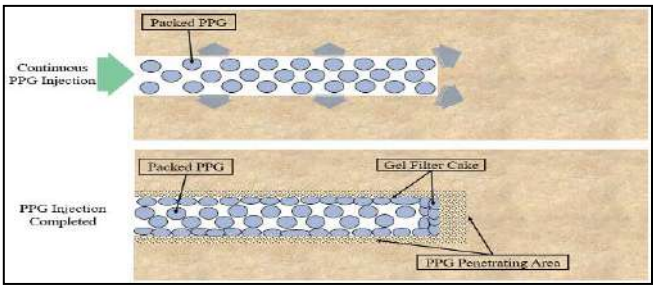

Fig. 3. Polymer Gel Plugging Mechanism in Fractures with tips (Polymer gel forms cake on rock surface and form impermeable layer that can block water flow from fractures)

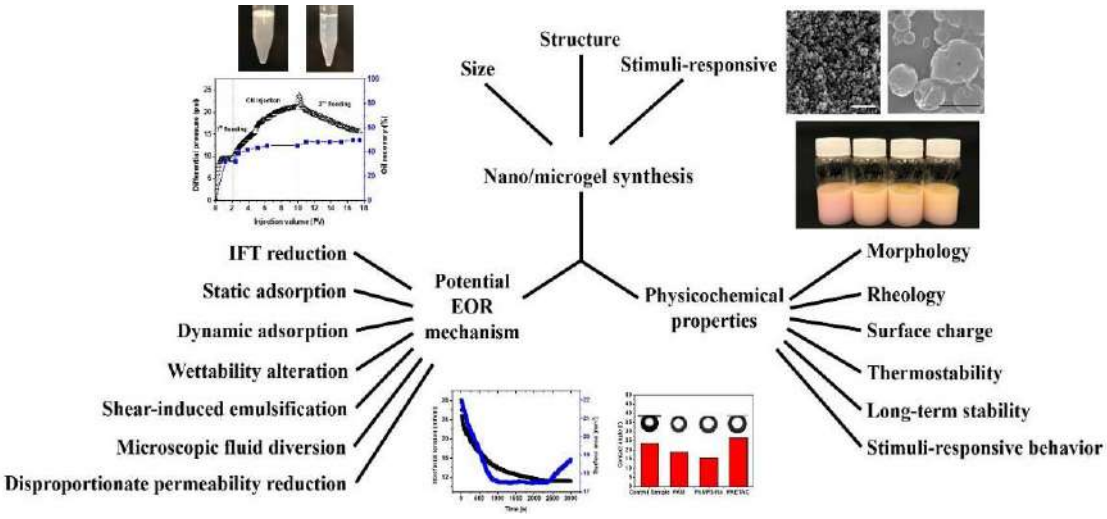

Fig. 4. EOR Mechanisms of Nanogels

Characterize Shale and Tight Gas Rock and Investigate Multiple Phase Flow Behavior in Nano-Scale Pore Space and Crack. To improve the understanding of the flow behavior of natural gas and introduced fluids (water, surfactant solutions and polymers) in nano-darcy range of tight gas and shale formations, Dr Bai was funded a project titled "Using Single-molecule Imaging System Combined with Nano-fluidic Chips to Understand Fluid flow in Tight and Shale Gas Formation" by RPSEA/DOE. This fundamental research has been completed by a multiple-disciplinary research group using integrated methodologies, including: (1) using multiple techniques to characterize the petrophysics properties of shale and tight rock samples and reconstruct their 3D pore structure; (2) using novel nanofluidic chips and single molecule detection technologies to physically visualize fluid flow behavior in nanometer-sized pores and cracks through lab experiments (Figure 4) ; (3) running imbibitions and core flooding tests to understand the effect of hydraulic fluid compositions on the petrophysics properties of shale and tight rocks; (4) developing pore scale numerical simulation to provide information that cannot be easily obtained from nanofluidic chip experiments and core flooding tests, such as the three-dimensional motion of liquid-gas interfaces and transport of additives and inclusions. The fundamental research has resulted in novel methods to determine the fluid flow properties in tight and shale formation.

Representative Papers

1. Pu, J., Bai, B., Alhuraishawy, A., Schuman, T., Chen, Y., & Sun, X. (2018, September 24). A Novel Re-Crosslinkable Preformed Particle Gel for Conformance Control in Extreme Heterogeneous Reservoirs. Society of Petroleum Engineers. doi:10.2118/SPE 191697-MS.
2. Sun, X. Suresh, S., Zhao, X., Bai, B. (2018), Effect of supercritical CO2 on the dehydration of polyacrylamide-based super-absorbent polymer used for water management, *Fuel* 224, P 628-636, 2018.
3. Geng, J., Pu, J., Wang. L., Bai, B. (2018), Surface charge effect of nanogel on emulsification of oil in water for fossil energy recovery, *Fuel* 223, P140-149, 2018.
4. Alhuraishawy, A. K., Bai, B., Wei, M., & Almansour, A. (2018). Preformed Partial Gel Injection Chased by Low-Salinity Waterflooding in Fractured Carbonate Cores. *SPE Reservoir Evaluation & Engineering* Society of Petroleum Engineers. doi:10.2118/SPE 191364-PA.
5. Wang, Z., & Bai, B. (2018, December 1). Preformed-Particle-Gel Placement and Plugging Performance in Fractures With Tips. *SPE Journal* 23(8), 2316-2326, SPE193997-PA
6. Tongwa, P, Bai, B., (2015), Degradable nanocomposite preformed particle gel for chemical enhanced oil recovery applications, *Journal of Petroleum Science and Engineering* 124, 35-45, 2015.
7. Wu Q. , **Bai, B.**, Y Ma, JT Ok, X Yin, Neeves, K. (2014) Optic Imaging of Two-Phase-Flow Behavior in 1D Nanoscale Channels, SPE 164549-PA, *SPE Journal 19(05), 793-802*.
8. **Bai, B**.; Elgmati, M.; Zhang, H; Wei, M., (2013), "Rock Characterization of Fayetteville Shale Gas Plays," *Fuel*, 105, 645-652.
9. **Bai, B**.*, Li, L., Liu, Y., Li, Y., (2007) "Conformance Control by Preformed Particle Gel: Factors Affecting its Properties and Applications," *SPE Reservoir Evaluation and Engineering* 10 (4), 415-421. DOI: 10.2118/89389-PA
10. **Bai, B.*,** Liu, Y., Coste, J-P., (2007) "Preformed Particle Gel for Conformance Control: Transport Mechanism through Porous Media," *SPE Reservoir Evaluation and Engineering*, 10 (2), 176-184. DOI: 10.2118/89468-PA.

Human Spatial Cognition

by Stephen C. Hirtle, Member EUAS

Short Biography

Professor of Computing and Information, University of Pittsburgh, Pittsburgh, PA

Education

Ph.D., 1982, Psychology (Mathematical), University of Michigan, Ann Arbor, Michigan, M.A., 1980, Psychology, University of Michigan, Ann Arbor, Michigan
M.A., 1978, Mathematics, University of Michigan, Ann Arbor, Michigan
B.A., 1976, Psychology and Mathematics, Grinnell College, Grinnell, Iowa

Positions

1999-present	*Professor, School of Computing and Information, University of Pittsburgh*
2010	*Visiting Professor, Institute for Geoinformatics, Augsburg University, Germany*
2002	*Visiting Professor, School of Information Technology, Auckland Institute of Technology, New Zealand*
1995	*Visiting Professor, Department of Computer Science, Molde College, Molde, Norway*
1994-1995	*Visiting Professor, Department of Geoinformation, Technical University of Vienna, Vienna, Austria*
1989-1999	*Associate Professor, Department of Information Science, University of Pittsburgh*
1989	*Visiting Professor, Department of Psychology, University of Umeå, Umeå, Sweden*
1987-1989	*Assistant Professor, Department of Information Science, University of Pittsburgh*
1982-1987	*Assistant Professor, Department of Psychology, SUNY-Albany.*
1981	*Human Factors Intern, Bell Laboratories, Holmdel, New Jersey.*
1977-1981	*Research Associate/Senior Statistician, Mental Health Research Institute, Ann Arbor, Michigan*

Professional Activities

Editor, Spatial Cognition and Computation, 1998-2007.
Chair, Steering Committee of Conference on Spatial Information Theory (COSIT), 2009-present.

Journal Review and Editorial Boards:

Spatial Cognition and Computation, 2007-present.
The URISA Journal, 2000-present.
Book Review Editor, Journal of Classification, 1994-2000.
Editorial Board Member, Classification Literature Automated Search Service, 1994-present.
President, Classification Society of North America, 1999-2000.

Review Panels

Panelist for National Science Foundation IIS/CISE Review, NIH Methodology and Measurement in the Behavioral and Social Sciences, National Science Foundation Cyber-Enabled Discovery in the Cognitive and Social Sciences, National Science Foundation ITR, National Science Foundation SBIR review panel.

Program Committee Member:

AAAI Spring Symposium Series on Cognitive Shape Processing, ACM Hypertext, ACM International Symposium on Advances in Geographic Information Systems, ACM SIGSPATIAL GIS, AGILE: International Conference on Geographic Information Science, American Society for Information Science, Classification Society of North America, Cognitive Models of Dynamic Phenomena and Their Representations, Conference on Spatial Information Theory (COSIT), European Conference on Spatial Information Theory, GIScience, GISTAM, International Conference on GeoSpatial Semantics, International Federation of Classification Societies bi-annual meeting, Belgium, National Center for Geographic Information and Analysis (NCGIA), 1993-1997, RIAO 2007, Large-Scale Semantic Access to Content, Transactions in GIS Special Issue on Semantic Similarity Measurement and Geospatial Applications, Varenius Project, National Center for Geographic Information and Analysis

Research

The ability to orient in space, to navigate to a new location, and to later recall the directions to a previously visited locale is a remarkable skill that humans, and to a lesser extent other species, are able to accomplish using a variety of environmental cues. How does one know where they are located, in which direction to head if moving, what landmarks are important to notice to stay oriented, and how to avoid getting lost? At the heart of human navigation is the "what" and the "where" of objects in space and how to move among those objects, including one's present location. Directions vary greatly in precision and granularity, be it 'make your next right,' 'turn right onto Main Street in 200 meters,' 'turn right at the top of the hill just after the red house,' or simply 'head to the city center.' Choosing one of these simple statements encompasses a large number of cognitive, cultural, and environmental principles, as well as individual differences. As the world moves to ubiquitous navigation systems, the problems of usability reman, particularly for new environments, including indoor navigation.

Relevance and Granularity

In Hirtle, Timpf and Tenbrink (2011) route directions were customized based on the purpose of the navigation. Primary to our conceptualization is that the activity at hand constrains the relevance of spatial information for task performance, as well as the level of granularity at which information is needed. In this paper, we highlight the role of activity for relevance and granularity first based on a review of each of the components involved, and furthermore by a semantic analysis of content patterns in human-generated instructions. The analysis identifies the verbalization styles that are associated with distinct types of activities on the basis of individual keywords that may serve as indicators.

We offer a strong theoretical argument for the importance of activities and provide a first step towards an operationalization of this concept, as well as implications for the development of cognitively motivated navigation systems. The investigation of route directions has increasingly aimed at a systematic differentiation of conceptual aspects determining the choice of spatial components to be represented. Many accounts have jointly achieved the identification of a relatively constant set of cognitive elements that are used as building blocks in route directions, including start and end point, route segments, action and movement descriptions, reorientations, landmarks, regions and areas, and distances. Further research has highlighted different levels of granularity and an impact of considerations of relevance on the ways in which these elements are chosen and represented in a description.

We argue that these various influences can be comprehensively captured by understanding the activity at hand. To substantiate this claim, we first review previous

findings on relevance and granularity. The mix between the purpose and attributes can be seen in Table 1.

Table 1. Attributes of directions (columns) versus the purpose of navigation (rows)

	Time pressure	Beauty of landscape	Urban architecture	Effort	Focus on destination	Focus on the path
Getting somewhere urgently	+	o	o	-	+	o
Enjoying natural scenery	-	+	-	o	o	+
Educational trip / Sightseeing	-	o	+	o	+	+
Attending sporting event	o	o	o	o	+	o
Following trail for hiking or exercise	o	+	o	+	o	+

Personalized Directions

In Hirtle, Richter, Srinivas, and Firth (2010), the authors highlight that the granularity of spatial information for navigation assistance remains an interesting and challenging problem. While useful directions in well-known areas can be notably vague, such as “head towards the airport,” there are other situations where navigation requires great cognitive effort. By examining steps that were flagged as being particularly difficult in verbal route directions, we were able to determine when the granularity of the directions need to be increased, so that they are more detailed and even redundant. The steps that were judged to be the “tricky part” of the directions were due for the most part to ambiguous geometry within the road network, absence of appropriate signage or landmarks, the need for quick sequential decision, or unusual constraints on driving or turning.

It was shown that the different reasons for trickiness pose different challenges. Some of the challenges may be solved in actual implementations, while others are hard even on a theoretical level. In general, however, even with tricky parts being flagged, removing the securing phase from generating automated instructions and not providing any feedback mechanisms, as it is the case in today’s navigation services, will result in some failures in the navigation process. The most problematic steps in a navigational sequence were generally related to a violation of expectations that the traveler brings to bear on the navigation task. Thus, while aspects of difficulty can be resolved in current and future automated route guidance systems, the problem of counter-expectancy will prove to be a particular challenge for designers of automated systems.

Indoor Navigation

The navigation of complex indoor environments remains a burgeoning field of study with a growing number of empirical tools to monitor, model, and analyze navigational problems. As David Stea eloquently wrote in 1974, “The idea or image of a building is as important as the building itself”. This powerful thought has been implemented in a variety of research projects from observing confusions in wayfarers to using isovist and space syntax methods to model the information being extracted from the building.

The development of context-aware, adaptive navigation, be it for autonomous robots or human travelers in a new environment, are on the forefront of development. In doing so,

there are environmental cues, infrastructure issues and user preferences to bring to bear on the development of user-friendly indoor navigation systems. The focus of this work is based on the user-centered context of looking at capabilities, preferences, and interface issues. The modeling techniques of space syntax is but one possible modeling technique that can be used. Finally, one can look at the transition between indoor and outdoor spaces to complete the analysis. This division itself is not robust and recent work has examined transitional spaces.

In Hirtle (2018), the idea of modelling spatial cognition is reviewed with depth, beginning with review of the history of building computational models in the field of spatial cognition for the purpose of positing underlying cognitive mechanisms, defining appropriate parameters, and testing empirical results. Such models include, but are not limited to, computer simulation models, process models, symbolic models, connectionist models, topological models and mental models, which draw on the modeling practices in fields of cognitive psychology, geography, computer science, neuroscience, linguistics, and others. The chapter begins with a short overview of the development of models of spatial cognition, including the nature of modeling. This is followed by a detailed look at exemplar models in seven different areas (qualitative, synergistic, space syntax, robotic, symbolic, topological, and geographical), which highlight the diversity of approaches to modeling spatial cognition. Finally, the chapter ends with an annotated list of primary readings that should form the foundation of any future research in this area.

Building on this earlier framework, the state of the art in terms both theory and navigational aids was reviewed in Hirtle and Bahm (2015). The result of this analysis is an aggregated view of what makes indoor environments different from outdoor or transitional environments. This line of research endeavors to coalesce the known cognitive principles to guide further research and tools in indoor wayfinding. Combing several earlier lines of research, Hirtle (2018) examined how indoor navigation differs from outdoor navigation and finally, how these ideas can come together in the development of cognitively-motivated tools for wayfinding.

Representative Publications

Hirtle, S. C. (2018). Wayfinding and Orientation: Cognitive Aspects of Human Navigation. In Montello, D. (Ed.) *Handbook of Behavioral and Cognitive Geography*. Edward Elgar.

Bahm, C. R., & Hirtle, S. C. (2017). Global Landmarks in a Complex Indoor Environment. In Leibniz International Proceedings in Informatics, forthcoming.

Hirtle, S. C., & Bahm, C. R. (2015). Cognition for the navigation of complex indoor environments. In H. Karimi (Ed.) *Indoor Wayfinding and Navigation* (pp. 1-12). Boca Raton, FL: CRC Press.

Hirtle, S. C., & Bahm, C. R. (2015). Cognition for the Navigation of Complex Indoor Environments. In H. A. Karimi (Ed.) *Indoor Wayfinding and Navigation*, (pp. 1-12). CRC Press,.

Hirtle, S. C., & Raubal, M. (2013). Many to many mobile maps. In M. Raubal, D. Mark, & A. Frank (Eds). *Cognitive and Linguistic Aspects of Geographic Space: New Perspectives on Geographic Information Research* (pp. 141-157). Berlin: Springer.

Hirtle, S. C. (2012). Models of spatial cognition. In Waller, D. & Nadel, L. (Eds) *APA Handbook of Spatial Cognition.* Washington: APA Press.

Hirtle, S. C., & Robles, C. (2012). Environmental Matching with Limited Displays. Paper presented at the Workshop on Spatial Knowledge Acquisition with Limited Information Displays, Kloster Seeon, Germany, August 31, 2012.

Hirtle, S. C., Timpf, S., & Tenbrink, T. (2011). The effect of activity on relevance and granularity for navigation. *Conference on Spatial Information Theory, 2011*. Berlin: Springer.

Hirtle, S. C., Richter, K.-F., Srinivas, S., & Firth, R. (2010).This is the tricky part: When directions become difficult. *Journal of Spatial Information Science*, 1(1), 53-73.

Hirtle, S. C. & Srinivas, S. (2010). Enriching spatial knowledge through a multi-attribute locational system. In C. Hölscher, T. Shipley, M. Olivetti Belardinelli, J. Bateman & N. Newcombe (Eds.), *Spatial Cognition VII* (Vol. 6222, pp. 279-288). Berlin: Springer

Hirtle, S. C. (2010). Dinosaurs, slide rules and maps. Paper presented at Las Navas 2010: Cognitive and Linguistic Aspects of Geographic Space, July 4 - 8, 2010, Las Navas del Marques, Avila, Spain.

Conjugated Polymers & Carbon Nanomaterials for Energy-Related & Biomedical Applications

by Liming Dai, Member EUAS

Short Biography
Kent Hale Smith Professor
Director, Center of Advanced Science and Engineering for Carbon (Case4Carbon) Department of Macromolecular Science and Engineering
Case School of Engineering, Case Western Reserve University

Education:

Ph.D. in Chemistry, Australian National University, Australia, 1991.
B.Sc. in Polymer Materials Science and Engineering, Chemical Engineering, Zhejiang University, China, 1983.

Current Position:

August, 2009 – Present, Kent Hale Smith Professor; Department of Macromolecular Science and Engineering, Director, Center of Advanced Science and Engineering for Carbon, Case School of Engineering, Case Western Reserve University

Positions Held:

August, 2004 – August, 2009, Wright Brothers Institute Endowed Chair Professor of Nanomaterials and Professor of Chemistry, College of Engineering, University of Dayton, USA
March, 2002 – August, 2004, Associate Professor of Polymer Engineering, College of Polymer Science and Polymer Engineering, University of Akron, USA
October, 1992 – March, 2002, Principal Research Scientist, The Commonwealth Scientific and Industrial Research Organisation (CSIRO), Clayton, Australia
June, 1992 – October, 1992, Visiting Fellow, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Illinois, USA
June, 1990 – June, 1992, AFRC Postdoctoral Research Fellow, Cavendish Laboratory, University of Cambridge, Cambridge, U.K
Dec., 1986 – June, 1990, PhD Candidate, Australian National University, Australia
July, 1983 – Dec., 1986, Eng., Zhejiang Chemical Industry Research Institute, China

Short-bio:

Liming Dai joined Case Western Reserve University (CWRU) in fall 2009 as the Kent Hale Smith Professor in the Department of Macromolecular Science and Engineering. He is also director of the Center of Advanced Science and Engineering for Carbon (CASE4Carbon) at CWRU. Dr. Dai received a BSc degree from Zhejiang University in 1983, and a PhD from the Australian National University in 1991. He accepted a postdoctoral fellowship from the Cavendish Laboratory at the University of Cambridge, and two years later became a visiting fellow in Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. He spent 10 years

with the Commonwealth Scientific and Industrial Research Organization (CSIRO) in Melbourne, Australia. Before joining the CWRU, he was an associate professor of polymer engineering at the University of Akron and the Wright Brothers Institute Endowed Chair Professor of Nanomaterials at the University of Dayton.

Dr. Dai's expertise covers the synthesis, functionalization, and device fabrication of conjugated polymers and carbon nanomaterials for energy-related and biomedical applications. He has published about 500 scientific papers, and held about 30 issued/applied patents. He has also published a research monograph on intelligent macromolecules and 6 edited/co-edited books on carbon nanomaterials for advanced energy systems and biomedical applications. He is a Highly Cited Researcher (Chemistry, Materials; Clarivate Analytics, formerly, Web of Science).

Editors and Editorial Board Members:

Associate Editor, Nano Energy
Specialty Chief Editor (Energy Materials), Frontiers in Materials
Editor-in-Chief of the Journal of Chemical Engineering and Process Technology
Member of the Advisory Editorial Board of the Electrochemical Energy Reviews
Member of the Advisory Editorial Board of the Materials Today Energy
Member of the Advisory Editorial Board of the ACS Nano
Member of the Advisory Editorial Board of the Matter
Member of the Advisory Editorial Board of the NanoScience
Member of the Advisory Editorial Board of the InfoMat
Member of the Advisory Editorial Board of the ChemNanoMat
Member of the Advisory Editorial Board of Journal of Bioengineering and Bioelectronics
Member of the Advisory Editorial Board of the Materials Research Express
Editorial Advisory Board of Chemistry of Graphene
Editorial Advisory Board of the Journal of Molecular and Engineering Materials
Editorial Advisory Board of the Journal of Nano Energy and Power Research, Editorial Board Member of the *International Journal of Polymer Science*
Associated Editor of *Research Letters in Physical Chemistry*
Associate Editor, International Journal of Smart and Nano Materials
Senior Editor of the Journal of Molecular Engineering and Systems Biology

Selected Publications

Selected Books

1. Liming Dai "*Intelligent Macromolecules for Smart Devices: From Materials Synthesis to Device Applications*", Springer-Verlag: Berlin, 2004.
2. Liming Dai (Ed.) *"Carbon Nanotechnology: Recent Developments in Chemistry, Physics, Materials Science and Device Applications*", Elsevier: Amsterdam, 2006.
3. Wei Lu, Jong-Beom Baek, Liming Dai (Eds.) *"Carbon Nanomaterials for Advanced Energy Systems*", John Wiley &Sons: New York, 2015.
4. Mei Zhang, Rajesh Naik, Liming Dai (Eds) "*Carbon Nanomaterials for Biomedical Applications*", Springer: Berlin, 2015.
5. Chunyi Zhi, Liming Dai (Eds) "*Flexible Energy Conversion and Storage Devices*", Wiley-VCH, Weinheim, 2018.
6. Liming Dai (Ed.) "Carbon-Based Metal-Free Catalysts: Design and Applications", 2 Vol., Wiley-VCH, Weinheim, 2018.

Selected Refereed Journal Papers

1. L. Qu, L. Dai, M. Stone, Z. Xia, Z.L. Wang "Carbon nanotube arrays with strong shear binding-on and easy normal lifting-off" *Science* **2008**, *322*, 238.
   This paper describes the development of carbon nanotube-based gecko-foot-mimetic dry adhesives. With a gripping ability nearly ten times better than a real gecko – the new carbon nanotube dry adhesive could give artificial gecko feet the ability to tightly grip vertical surfaces while being easily lifted off perpendicularly when desired.

2. K. Gong, F. Du, Z. Xia, M. Dustock, L. Dai "Nitrogen-doped carbon nanotube arrays with high electrocatalytic activities for oxygen reduction" *Science* **2009**, *323*, 760.
   In this work, I discovered that the FePc-generated CNTs could act as a metal-free electrode to effectively catalyze oxygen reduction reaction, a key reaction for renewable energy technologies (*e.g.*, fuel cells, metal-air batteries). Furthermore, the carbon nanotubes generated from FePc via a CVD process pioneered by my group is among the first nitrogen-doped carbon nanotubes. My team further developed the first N-doped graphene as a new metal-free carbon catalyst (*ACS Nano* **2010**, *4*, 1321), leading to worldwide studies on doped carbon and other related doped materials for a wide range of applications even beyond energy and catalysis. pioneering work on the heteroatom-doped carbon materials opens a new field of carbon-based metal-free catalysts with numerous follow-up studies worldwide.

3. D. Yu, L. Dai "Self-assembled graphene/carbon nanotube hybrid films for supercapacitors" *The Journal of Physical Chemistry Letters* 1 (2), 467-470, 2010.
   Owing to their unique electrical properties and large surface area, graphene nanosheets (GNs) have emerged as a new class of promising electrode materials attractive for potential applications in actuators, solar cells, field-emission devices, field-effect transistors, supercapacitors, and batteries. However, much of the surface area of GNs in the pristine graphene electrodes is lost due to graphene aggregation. For the first time, my group has used 1D carbon nanotubes (CNTs) to physically separate 2D GNs to preserve graphene's high surface area. This concept has subsequently been used to reduce the graphene aggregation around the world.

4. L. Qu, Y. Liu, J.B. Baek, L. Dai "Nitrogen-doped graphene as efficient metal-free electrocatalyst for oxygen reduction in fuel cells" *ACS Nano* **2010**, *4*, 1321-1326.
   This work demonstrates the first N-doped graphene as a new metal-free carbon catalyst, leading to worldwide studies on doped graphene and other related doped materials for a wide range of applications beyond catalysis.

5. J. Zhang, Z. Zhao, Z. Xia, L. Dai "A metal-free bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions" *Nature Nanotechnology* **2015**, *10*, 444-452.
   This paper describes the development of a low-cost and scalable approach to prepare three-dimensional mesoporous carbon foams as the first ORR and OER bifunctional carbon catalyst as the air electrode for both primary and rechargeable Zn-air batteries. This work has directly paved the way for other researchers to develop bi-/multi-functional carbon-based metal-free catalysts for energy device/system applications, a very hot research topic nowadays.

6. D. Yu, K. Goh, H. Wang, L. Wei, W. Jiang, Q. Zhang, L. Dai Y. Chen "Scalable synthesis of hierarchically-structured carbon nanotube-graphene fibres for capacitive energy storage" *Nature Nanotechnology* **2014,** *9*, 555.
   In collaboration with Prof. Yuan Chen at NTU (now Sydney University), we developed a simple, hydrothermal-assisted self-assembling process for scalable production of all carbon hybrid-fibers for flexible solid-state micro-supercapacitors with the highest specific volumetric energy density among the fiber-shaped supercapacitors.

7. J. Shui, M. Wang, F. Du, L. Dai "N-doped carbon nanomaterials are durable catalysts for oxygen reduction reaction in acidic fuel cells" *Sci. Adv.* ***2015****, 1, e1400129.*
   This work successfully demonstrates the use of metal-free catalysts in acidic polymer electrolyte membrane fuel cells, which is the mainstream fuel cell technology. My group showed that nitrogen-doped carbon nanotubes and their graphene composites catalyze oxygen reduction in these practical fuel cells with both excellent activity and durability. This work offers an inexpensive alternative to metal-based catalysts, which could dramatically reduce the manufacturing cost of fuel cells and open the door for their commercialization.

8. L. Dai, Y. Xue, L. Qu, H.J. Choi, J.B. Baek "Metal-free catalysts for oxygen reduction reaction" *Chemical Reviews* **2015**, *115*, 4823-4892.
   This invited article provides a concise and critical review on the rapidly developing field of metal free catalysts which could overtake metal-based catalysts in the race to the renewable energy technological marketplace. This is the first comprehensive review of this important topic and laid down the foundation for the field of carbon-based metal-free catalysts.

9. K. Lu, Z. Hu, J. Ma, H. Ma, L. Dai, J. Zhang "A rechargeable iodine-carbon battery that exploits ion intercalation and iodine redox chemistry" *Nature Communications* ***2017****, 8, 527.*
   By using a free-standing, flexible N,P-codoped porous carbons encapsulated with Li or Na and I ions as an anode, an iodine-carbon rechargeable batteries even without a Li or Na anode was developed, which exhibited excellent performance with a good cycling stability. The methodology developed in this study opens new avenues for the development of novel rechargeable batteries, even free from the metallic Li/Na anode and associated safety risks, from low-cost heteroatom-doped porous graphitic carbon via the combination of redox capacitive properties and ion intercalation.

10. L. Xue, Y. Li, X. Liu, Q. Liu, J. Shang, H. Duan, L. Dai, J. Shui "Zigzag carbon as efficient and stable oxygen reduction electrocatalyst for proton exchange membrane fuel cells" *Nature Communications* **2018**, *9, 3819*.
    This work demonstrates that zigzag carbon is a promising electrocatalyst for low-cost and durable proton exchange membrane fuel cells, indicating a great potential for graphitic carbon with defects to be used in PEM fuel cells.

Improvements in Cardiovascular Research & Echocardiography

by Thomas F. Lüscher, Member EUAS

Short Biography

Training and Current Position

Professor Lüscher studied medicine at the University of Zurich and obtained the board certification in internal medicine and cardiology. He trained in cardiovascular research and in echocardiography at the Mayo Clinic in Rochester, MN, USA and was later Professor of Pharmacotherapy at the University of Basel, then trained in interventional cardiology and became Professor of Cardiology at the University of Berne, before assuming a position as Professor and Chairman of Cardiology and Director of the University Heart Center at the University Hospital Zurich and Director of the Center for Molecular Cardiology at the University of Zurich, Switzerland. He is now Director of Research, Education & Development and Consulting Cardiologist at the Royal Brompton & Harefield Hospital Trust and the Imperial College in London.

Clinical Competence and Activity

Professor Lüscher is an active general and interventional cardiologist with a broad clinical scope and large experience in prevention, coronary and valvular heart disease, per-cutaneous interventions and heart failure. He has sucessfully taken care of cardiac patients for several decades from many countries.

Research

Professor Lüscher has been a mentor of numerous physicians and scientists. His research is translational in nature and focuses on vascular disease, specifically on the role of endothelium-derived mediators in the regulation of vascular tone and structure, platelet-vessel wall interactions, coagulation in aging, hypertension, lipid disorders and atherosclerosis. More recently, inflammatory pathways in these conditions and particularly in acute coronary syndromes has been at the center of his interest. He has published extensively, authoring or co-authoring over 500 original research articles and more than 200 reviews, book chapters and monographs including the ESC Textbook of Cardiovascular Medicine.

Recognition and Awards
By the Institute for Scientific Information he has been rated as one of the 0.5% most cited scientists worldwide. He has obtained numerous research prizes and prestigious lecturerships worldwide. He is a member of many editorial boards and was Associate Editor Europe of Circulation from 2004 to 2008. Since 2009 he is chairman of the publications committee of the European Society of Cardiology (ESC) and an ex-officio member of the ESC board as well as editor-in-chief of the European Heart Journal.

Research Topics

Professor Lüschers research is translational in nature and focuses on arteriosclerosis and coronary artery disease, specifically on the role of endothelium-derived mediators in the regulation of vascular tone and structure, platelet-vessel wall interactions, coa-gulation and on the effects of aging, hypertension, lipid disorders and diabetes on these pathways. He has pioneered endothelial function in human blood vessels and characterized the mechanisms and contribution of different endothelial mediators such as nitric oxide, prostaglandins, reactive oxygen species and endothelin in endothelial dysfunction in aging, hypertension, hyperlipidemia and diabetes. Aging and longevity genes such as the adaptor protein $p66^{shc}$, the transcription factor JunD and the Sirtuin family have been shown by his group to markedly affect endothelial function and me-diate the effects of cardiovascular risk factors in the vessel wall as silencing or acti-vation, respectively of these genes modulates profoundly endothelial function, the first step in the atherosclerotic process. Several clinical studies have assessed the effects of cardiovascular drugs such as calcium antatonists, angiotensin converting enzyme inhibitors, angiotensin receptor and endothelin anatagonsist in different patient popu-lations such as those with hypertension, diabetes, hyperlipidemia coronary artery disease and heart failure.

Another interest was the biology of high-density lipoprotein cholesterol (HDL-C). Of note, while HDL-C is protective in vascular cells and at an epidemioogical level, all attempts to improve outcome with drugs increasing its plasma levels have failed. Within a Leducq Network, he could show together with his transatlantic collegues that HDL-C becomes dysfunctional as patients become hypertensive, diabetic, have coronary artery disease or even an acute myocardial infarction or renal failure. This concept of HDL-C dysfunction could later be confirmed in clinical studies in patients with coronary artery disease using HDL-C elevating drugs or HDL-C analogues which all had a neutral or even damaging effect on vascular function or outcome.

More recently, inflammatory pathways in coronary artery disease and

particularly in acute coronary syndromes has been at the center of his interest. To that end, inflam-matory markers such as cytokines and chemokines and cellular receptors such a Toll-like receptors have been characterized in patients with an acute coronary occlusion in the catheterization laboratory using samples directly from occluded coronary arteries. Importantly, interleukin-6 among other cytokines is highly overexpressed at the site of coronary occlusion demonstrating the importance of local inflammation on the develop-ment of plaque rupture and myocardial infarction. This finding was recently confirmed in the CANTOS trial as a major predictor of the beneficial effects of interleukin-1 blockade as those with markedly reduced interleukin-6 levels had the largest clinical benefit. These acute findings were then translated into clinical studies evaluating pro-gnostic biomarkers in these patients. As such novel markers such as Cyr61 and meta-bolites of the microbiome such as trimethylaminooxid, trimethly lysine and carnitine metaboites have been shown to be potetn and novel prognostic markers beyond currently used risk scores.

Lastly, a new acute coronary syndrome, the Tako Tsubo Syndrome attracted his atten-tion. With a large international registry, the InterTAK registry, he could show with his team that the Tako Tsubo Syndrome is primarily affecting postmenopausal women and is not a harmless disease as it is associated with a 4% acute mortality and a 15% rate of cardiogenic shock. In collaboration with neurophysiology collegues this team was able to show that such postmenopausal women have altered midbrain structures and function, particularly affecting the amygdala and hippocampus. This may explain why such patients have massive sympathetic activation and activation of endothelin during acute events triggered by either psychological or physical factors. This in turn may lead to coronary microvascular constriction and left ventricular dysfunction with apical ball-ooning and acute heart failure and potentially death.

Professor Lüscher has published his findings extensively in peer reviewed prestigious journals, authoring or co-authoring over 500 original research articles and more than 200 reviews, book chapters and monographs including the *ESC Textbook of Cardio-vascular Medicine*. By the *Institute for Scientific Information* he has been rated as one of the 0.5% most cited scientists worldwide. He has obtained numerous research prizes and prestigious lecturerships worldwide.

Mentoring

Professor Lüscher has mentored several hundred fellows in basic science and clinical cardiology. Many of them are now independent and successful scientists or

physicians, some are now even professors and chaipersons of departments or chiefs of medical services or editors of scientific journals.

Editorships

Professor Lüscher is a member of many editorial boards and was Associate Editor Europe of *Circulation* (Journal of the American Heart Association) from 2004 to 2008. Since 2009 he is chairman of the publications committee of the *European Society of Cardiology* (ESC) and an ex-officio member of the ESC board as well as editor-in-chief of the *European Heart Journal*, currently the Nr. 1 journal in cardiovascular medicine with an impact factor of 23.425. Furthermore, together with John A. Camm, Gerald Maurer and Patrick W. Serruys he is editor of the *ESC Textbook of Cardiovascular Medicine* and of its electronic version *ESC CardioMed*.

Science and Technology of a Multifunctional Oxide and Nanocarbon Thin Films & Application to Development and Commercialization of a New Generation of Multifunctional Devices

by Orlando Auciello, Member EUAS

Short Biography

Orlando Auciello is Distinguished Endowed Chair Professor at the University of Texas-Dallas (Materials Science/Engineering and Bioengineering Departments, 2012 - present)

Auciello graduated with M.S. (1973) and Ph.D. (1976) degrees in Physics from the Physics Institute "Dr. Balseiro" (Universidad Nacional de Cuyo, Argentina). Electronic Engineering at the University of Cordoba-Argentina (1964-1970).

Auciello was Postdoctoral at Mc Master University (Canada, 1976-1979), Research Scientist at the University of Toronto-Canada (1979-1984), Associate Professor at North Carolina State University (1985-1988), Senior Research Scientist at the Microelectronics Center of North Carolina (1988-1996), Senior Scientist (1996-2005) and Distinguished Argonne Fellow (2005-2012).

Auciello is directing basic and applied research programs on different fields, involving multi-component oxide thin films and application to systems and devices (ferroelectric memories, high-k dielectric oxide films, resistive change memories, nanoscale CMOS devices, photovoltaic energy generation / super-capacitors for energy storage devices, high-frequency devices, piezoelectric thin films for MEMS/NEMS sensors and actuators); and nanocarbon thin films (ultrananocrystalline diamond (UNCD), nanocrystalline diamond (NCD), and microcrystalline diamond (MCD) and graphene films) and applications to industrial, high-tech and medical devices. Auciello's work on ferroelectric films contributed to the development of nonvolatile memories now in the market in smart cards.

The UNCD film technology developed and patented by Auciello and colleagues is now commercialized by three companies co-founded by him and colleagues:

• Advanced Diamond Technologies (ADT), spun-off from Argonne National Lab (top company spun-off from a DOE Laboratory) in 2003 (Profitable in 2014) is commercializing industrial components and systems (UNCD-coated mechanical pump seals and bearings, and water purification systems based on electrolysis with corrosion resistant electrodes based on electrically conductive B-doped UNCD-coated metal electrodes) (Auciello is co-founder, equity holder, investor, and working closely to develop new UNCD coated industrial products for ADT).

• Original Biomedical Implants (OBI)-USA in 2013, and OBI-Mexico in 2016, for developing and commercializing a new generation of UNCD-based high-tech and implantable medical devices and medical treatments based on nanotechnology. Products in advanced state of development by OBI-USA and OBI-Mexico include: i) new generation of Li-ion batteries with anodes, cathodes, membranes, and inner walls of battery cases coated with corrosion resistant UNCD coatings, enabling LIBs with ≥ 10x longer life and safer than current LIBs, for applications to defibrillators/pacemakers, cell phones, computers, battery-powered electronic devices, and electric cars; ii) Biocompatible UNCD-coated dental implants with practically no corrosion induced in current metal-based dental implants by oral fluids; iii) UNCD-coated metal prostheses (hips, knees) with no failure due to the protective UNCD coating; iv) new retina reattachment procedure,

using biocompatible super-paramagnetic nanoparticles injected inside the eye attracted by an external temporary magnet to push the retina back into place (clinical trials performed in Argentina between 2015-2106 restored full vision to two patients (2 patents granted in USA and Japan in 2016).
Auciello has published 20 books and about 500 articles in the fields described above, holds 25 patents, and organized, chaired, and lectured at numerous national and international conferences. He is associate editor of Appl. Phys. Lett., Integrated Ferroelectrics, and editor of two book series on thin films and applications to devices (Academic Press). He was member of the Materials Research Society (MRS) Board of Directors (2000-2003), Chair of the MRS International Relations Committee 2005-2010, ***Vice President of the MRS (2012), President of the MRS (2013), and Past President of the MRS (2014).***
He has numerous Awards, including seven R&D 100 Awards, 2003 Hispanic Engineering National Achievement Award, 2006 Federation of National Laboratories Award, 2008 University of Chicago Distinguished Performance Award, and is a ***Fellow of the AAAS and MRS.***

Science and Technology on Multifunctional Oxide Films

1986-1996. O. Auciello (NCSU and MCNC) and colleagues were one of the first two groups in producing Y-Ba-Cu-O High Temperature Superconductors (HTSC) Films based on the bulk YBCO material discovered in the late 1980's, which earned the Noble Prize to two European scientists. This work opened the way for an intensive research on the science and technology of high temperature superconducting thin films from the 90's until today.
J. Narayan, N. Biunno, R. K. Singh, O.W. Holland, and **O. Auciello**, "Formation of Thin Superconducting Films by Laser Processing Method," Appl. Phys. Lett. **vol. 51** (1987) 1845-1847.
ISI Citation Information: Times Cited: 500

O. Auciello, A.R. Krauss, J. Im, and J.A. Schultz "Studies of Multicomponent Oxide Films and Layered Heterostructure Growth Processes via in situ, Time-of-Flight Ion Scattering and Direct Recoil Spectroscopy,", Annual Rev. of Materials Science, **vol**. **28 (1998) 375**-396
Importance: this paper showed the importance of the *in situ* ion scattering characterization technique to study the growth of oxide and other films in relatively high pressure environments, while before the ion scattering technique could be used only in high vacuum, not allowing to study film growth processes in situ/real time.

1986-2008. O. Auciello (NCSU and ANL) and colleagues pioneered the development of conducting oxide electrodes (RuO_2 was patented as the first oxide electrode for Ferrolectric Random Access Memories (FeRAMS) to eliminate the 30-year old problem of polarization fatigue in $PbZr_xTi_{1-x}O_3$ (PZT) ferroelectric capacitors for FeRAM, through a careful control of oxygen vacancies at the electrode-ferroelectric interface. This was a critical step in the development of reliable FRAMs based on PZT thin films. Fujitsu and Texas Instruments are currently using the conducting oxide electrode approach for commercialization of FeRAMs based on PZT thin films **(1986-1996**).

A.I. Kingon, **O. Auciello**, H.N. Al-Shareef, D.J. Lichtenwalner, and R. Dat,"Hybrid Metal / Metal-Oxide Electrodes for Ferroelectric Memories," US Patent #5,555,486; (1996).

O. Auciello, J.F. Scott, R. Ramesh, "The Physics of Ferroelectric Memories," July (1998) p. 22.
ISI Citation Information: Times Cited: 1000
Importance: this paper showed the physics and future of ferroelectric memories for insertion in the market.
Latter on, **in the 2000s**, Auciello and colleagues conducted pioneering research, using the unique one of two worldwide highest energy/intensity X-Ray synchrotron (Advanced Photon Source-Argonne National Laboratory) to demonstrate that the limit of ferroelectricity in Perovskite PbTiO Films is three Atomic Units. This R&D opened the way for the science and technology of nanoferroeletrics.

D.D. Fong, G.B. Stephenson, S.K. Streiffer, J.A. Eastman, **O. Auciello**, P.H. Fuoss, C. Thompson, "Ferroelectricity in Ultrathin Perovskite Films," Science, **vol. 304** (2004) 1650-1653. **ISI Citation Information: Times Cited: 500**

1995-present. O. Auciello and A. Gruverman demonstrated the use of a new technique (Piezoresponse Force Microscopy-PFM) based on Atomic Force Microscopy to study ferroelectric domain configuration and dynamics at the nanoscale in ferroelectric thin films. This technique is based on measuring the atomic scale displacement of the atoms on the surface of the ferroelectric materials upon application of a voltage between the top and bottom surface of the ferroelectric layer which induces the polarization and associated piezoelectric (i.e., physical displacement of ions in the lattice) phenomena. Many groups now use this technique worldwide, and several companies are commercializing AFM-PFM systems for research.

A. Gruverman, **O. Auciello,** and H. Tokumoto "Imaging and control of domain structures in ferroelectric thin films via scanning force microscopy,", Annual Rev. of Materials Sience, **vol. 28**, (1999) 101-123,
ISI Citation Information: Times Cited: 400.
Importance: this paper showed the importance of the new piezoresponse imaging technique to study ferroelectric domains at the nanoscale and open the new field of PFM imaging of ferroelectric domains and contributed to develop a new market of PFM instrumentation.

1996-present O. Auciello pioneered the development of a unique multifunctional material in thin film form. The material is based on a novel TiAl alloy layer, for which Auciello's group demonstrated several functionalities, namely: 1) oxygen diffusion barrier to integrate oxides (e.g., $BaSr_xTi_{1-x}O_3$ (BST)) films (grown at high-temperature in oxygen-rich environments) with copper electrode layers (without oxidation of the electrode) to achieve the highest performance BST based capacitors with the highest electrical conductivity electrodes for high frequency devices demonstrated today; Auciello's group used more recently the same TiAl barrier to integrate oxide piezoelectric thin films with a novel multifunctional material in thin film form, named ultrananocrystalline diamond (UNCD), to develop a new generation of low voltage piezoelectrically actuated diamond microelectromechanical/ nanoelectromechanical systems (MEMS/NEMS) with the highest performance demonstrated today; the observation that TiAL formed a thin oxide layer (~3 to 4 nm thick) lead to another breakthrough functional use of TiAl alloys, in this case as an amorphous $TiAlO_x$ layer with relatively high-dielectric constant and bandgap for application as a novel amorphous high-k dielectric to replace SiO_2 ion the next generation of nanoscale CMOS devices. The idea came from observing that Al_2O_3 is the material with the highest bandgap (~ 8 ev)) closest to SiO_2 (~ 9 eV), although with relatively low K- 10, while TiO_2 exhibits the highest K among all amorphous oxides being explored for the new generation of high-K CMOS gates, but with relatively low bandgap (3.3 eV). Based on this observation, Auciello postulated that by producing a $Ti_xAl_{1-x}O_3$ with the appropriate stoichiometry, this material can provide a better alternative to HfO_2, which is currently the material that replaced SiO_2 in every CMOS device in the market today.

O. Auciello, W. Fan, B. Kabius, S. Saha, and J.A. Carlisle, C. Lopez and E.A. Irene, R.A. Baragiola "A New Hybrid $Ti_xAl_{1-x}O_y$ Gate Dielectric Layer for Next Generation Ultra-High Capacitance Density CMOS Gates,", Appl. Phys. Lett **86** (2005).
Importance: this paper demonstrated that the new TiAlOx dielectric layer exhibits the highest dielectric constant (~ 35) among all known amorphous oxides, including HfO_2, which replaced SiO_2 in CMOS devices in 2006.

Following the R&D on $Ti_xAl_{1-x}O_3$ films described above, Auciello's group pioneered another breakthrough in
the high-K dielectric thin film field, which consisted in the development of a new material science approach based on growing $TiOx/Al_2O_3$ nanolaminates (NLs) that produced he highest dielectric constant oxide thin films known today. For 150 nm thick $TiOx/Al_2O_3$ NLs with sub-nanometer thick sublayers, few Angstrom change in sublayer thickness dramatically increases relaxation cut-off frequency by more than 3 orders of magnitude with high dielectric constant (k> 800). This unusual phenomenon was demonstrated to be based on the two-phase Maxwell-Wagner relaxation phenomena.

G. Lee, B-K Lai, C. Phatak, R.S. Katiyar, and **O. Auciello**, "Tailoring Dielectric Relaxation in Ultra-Thin High-Dielectric Constant Nanolaminates for Nanoelectronics", Appl. Phys. Lett **102** (2013) 142091.

W. Li, Z. Chen, R. N. Premnath, B. Kabius, and **O. Auciello**, "Controllable Giant Dielectric Constant in Al_2O_3/TiO_2 Nanolaminates", J. Appl. Phys. **110** (2011) 024106-1-8.
Importance: The two papers cited above open the way for the new field of science and technology of multifunctional oxide nanolaminates.
The concept of $TiOx/Al_2O_3$ nanolaminates was subsequently extended by Auciello's group to investigate and develop $BiFeO_3$ (BFO)/ $SrTiO_3$ (STO)/BFO nanolaminates (BSB-NLs) featuring nanometer-scale thickness of BFO and STO layers. By introducing the STO layer in between two BFO layers, the leakage current density was reduced by two orders of magnitude with respect to relatively high leakage currents of single BFO layers, i.e., from 10^{-5} A/cm^2 to 10^{-7} A/cm^2. The BSB-NL also shows very high piezoelectric response, which is ~ 5 times higher than that of the pure BFO with the same thickness. The highly strained state of the BFO layers concurrently with the chemical/crystallographic state of the interfaces between the BFO and STO layers contribute to the very high values of piezoresponse and very low leakage current observed in the BSB-NLs.

G. Lee, E. M. A. Fuentes-Fernandez, G. Lian, R. S. Katiyar, and **O. Auciello**, "Hetero-epitaxial $BiFeO_3/SrTiO_3$ Nanolaminates with Higher Piezoresponse Performance Over Stoichiometric $BiFeO_3$ Films", Appl. Phys. Lett. **106**, (2015) 022905.

Importance: this paper opened the way for a new field focused on R&D on piezoelectric nanolaminates with superior piezolectric properties over those of single phase BFO films.

1996-present. O. Auciello and two colleagues (D. M. Gruen and A. R. Krauss) started a whole new field of research and technological development focused on the science and technology of a novel material in thin film form defined as ultrananocrystalline diamond (UNCD). They developed a unique patented plasma chemistry involving Ar (the lowest cost inert gas) and CH_4 as the source of C atoms to grow diamond films with the smallest grains demonstrated today (2-5 nm). UNCD films exhibit a unique combination of exceptional mechanical, tribological, physical, chemical, electronic, thermal transport, and biocompatible properties. They performed pioneering research to understand the fundamentals underlying the growth and the properties of UNCD, and in the process obtained several key patents to enable the commercialization of the UNCD technology. Auciello lead the work to demonstrate that UNCD films can be used in a wide range of technologies, and to do so, he co-founded Advanced Diamond Technologies (ADT) in 2004, jointly with J.A. Carlisle The multifunctionalities of UNCD enables a broad range of commercial applications, namely: a) UNCD coatings are now in commercial mechanical pump seals (marketed by ADT), making a major impact in enabling pumps in the chemical, the oil and car industries run with 20% savings in energy usage; b) Atomic Force Microscope UNCD tips now in the market provides wear-free AFM tips for much higher resolution AFM analysis as compared with wear prone Si tips; c) New diamond-based MEMS/NEMS technologies to replace the current Si-based technology that is hindering the development and commercialization of MEMS and NEMS devices, due to the poor mechanical and tribological properties of Si (new RF MEMS switches, using UNCD as a dielectric with controlled charging have been developed and are in the process of being inserted in a new generation of RF communication devices, electronic radars and more); d) New UNCD-based field electron emission cathodes for application to field emission displays, cold cathodes for mass spectrometer for deep space exploration and more ; e) Use of UNCD films as hermetic bioinert/biocompatible coating for encapsulation of Si microchips for implantable biomedical devices (a Si chip coated with UNCD will be implanted inside the eye as an artificial retina to restore sight to people blinded by retina degeneration)-the chip has been implanted on 31 blind people in the USA, England, France, Switzerland, and Mexico, and they are staring to read large letters and recognize objects again, although diffusively, because the current small number of electrodes (62-240) that inject electrical pulses from the chip image processed from a CCD camera on the ganglion cells for transmission to the brain to form images); f) Auciello's group recently demonstrated that UNCD surfaces support an efficient growth of stem cells, and they are now

investigating the feasibility of differentiating those cells into photoreceptors to replace the dead photoreceptors in the retina of people blinded by the death of photoreceptors, and in the future differentiation into spinal cord cells to eventually restore motion to people paralyzed by trauma of those cells, brain cells, to control or eliminate brain degradation conditions, such as Parkinson decease, and improvements in many other human conditions. This research started a new field of developmental biology based on the UNCD biocompatibility; g) Auciello is now directing R&D focused on developing a new generation of UNCD-coated metal-based prostheses (dental implants, hips, knees and many others), for which the biocompatible/body fluids corrosion resistant/lowest coefficient of friction UNCD coating eliminates the degradation produced in current metal-based prostheses, which require early than desired replacement. The new UNCD-coated implantable medical devices will produce a revolution in that industry worldwide.

W. Yang, **O. Auciello**, J.E. Butler, W. Cai, J.A. Carlisle, J.E. Gerbi, D.M. Gruen, T. Knickerbocker, T. Lasseter, J.N. Russell, L. M. Smith, R. J. Hamers "DNA Modified Nanocrystalline Diamond Thin Films as Stable, Biologically, Active Substrates,", *Nature Mater*. **1** (2002) 253-257.
Importance: This is the first paper that demonstrated that the surface of UNCD films can be functionalized to express DNA and other biomolecules, opening the field of diamond-based developmental biology.

X. Xiao, J. Birrell, J.E. Gerbi, **O. Auciello** and J.A. Carlisle, "Low Temperature Growth of Ultrananocrystalline Diamond," J. Appl. Phys. 96 (2004) 2232-2239.
Importance: This is the first paper that demonstrated that the UNCD films are the only diamond films that can be synthesized at 400 ˚C, opening the pathway to using UNCD for fabrication of monolithically integrated diamond MEMS/NEMS with CMOS devices to enable a whole new hybrid diamond MEMS/NEMS /CMOS technology.

S. Sudarsan, J. Hiller, B. Kabius, and **O. Auciello**, "Piezoelectric/Ultrananocrystalline Diamond Heterostructures for High-Performance Multifunctional Micro/Nanoelectromechanical Systems," Appl. Phys. Lett. **90** (2007) 134101.
Importance: this is the first paper demonstrating the possibility of integrating an oxide based piezoelectric film (PZT) with a carbon based material (UNCD) to produce a new generation of high-performance piezoelectrically actuated diamond MEMS/NEMS, opening the way for a new generation of advanced MEMS/NEMS devices driven by CMOS.

"*In Vitro* and *In Vivo* Evaluation of Ultrananocrystalline Diamond for Coating of Implantable Retinal Microchips," X. Xiao, J. Wang, J. A. Carlisle, B. Mech, R. Greenberg, R. Freda, M. S. Humayun, J. Weiland, and **O. Auciello**, J. Biomedical Materials **77B (2)** (2006) 273-281.
Importance: This paper demonstrated that UNCD coatings can enable the implantation of a Si microchip in the human eye as the key component of an artificial retina to restore sight to people blinded by retina photoreceptors' degeneration.

B. Shi, Q. Jin, L. Chen and **O. Auciello,** "Fundamentals of ultrananocrystalline diamond (UNCD) thin films as biomaterials for developmental biology: Embryonic fibroblasts growth on the surface of (UNCD) films," Diamond and Related Materials, **vol. 18** (2-3), (2009) 596-600.
Importance this is the first paper that demonstrates that UNCD surfaces are excellent for growing stem cells, thus opening the field for developmental biology based on diamond.

O. Auciello, P. Gurman, M. B. Guglielmotti, D.G. Olmedo, A. Berra and M. J. Saravia, "Biocompatible Ultrananocrystalline Diamond Coatings for Implantable Medical Devices", MRS Bulletin, vol. 39 (07) (2014) 621 – 629.

O. Auciello, "Novel Biocompatible Ultrananocrystalline Diamond Coating Technology for a New Generation of Medical Implants, Devices, and Scaffolds for Developmental Biology", Biomaterials and Medical Applications Journal, **vol 1** (1) (2017) 1000103.

Urban Spatial Structure & Transportation

by Qing Shen, Member EUAS

Short Biography

Professor, Department of Urban Design and Planning
Chair and Director, Interdisciplinary Ph.D. Program in Urban Design and Planning
University of Washington
Seattle, USA

Education

1993 *Ph.D. in City and Regional Planning, University of California, Berkeley, USA*
1986 *M.A. in Urban Planning, University of British Columbia, Canada*
1982 *B.E. in Architecture, Zhejiang University, China*

Employment

2009- *Professor, University of Washington; Department Chair, 2009-2014*
2006-2009 *Professor, University of Maryland, College Park; Associate Dean for Academic Affairs, School of Architecture, Planning, and Preservation, 2007-2009*
2001-2006 *Associate Professor, University of Maryland, College Park*
1999-2001 *Associate Professor, MIT*
1993-1999 *Assistant Professor, MIT*

Visiting Appointments

2015- *Oversea Dean (visiting), Southwest Jiaotong University, China*
2015-2017 *Peng Cheng Chair Professor (visiting), Peking University-Shenzhen, China*
2009-2012 *Tongji Chair Professor (visiting), Tongji University, China*
2005-2008 *Siyuan Chair Professor (visiting), Nanjing University, China*

Research Interests

Urban Spatial Structure
Urban Transportation Planning and Policy

Publications

Have authored or co-authored over 100 publications, including journals articles, book chapters, working papers, and project reports

Student Advising

Have supervised, as committee chair or committee member, over 30 Ph.D. dissertations and 60 Master's theses

Editorial Boards

Current editorial board member for 6 academic journals, including Journal of the American Planning Association (since 2000), Journal of Planning Education and Research (since 2006), and Journal of Transport and Land Use (since 2007)

Academic Services

Have served on scientific/organizing committees for many academic conferences;
Have played leadership roles in professional organizations, such as Chair of the International Association for China Planning and Chair of the Karen R. Polenske Scholarship Fund;
Have reviewed numerous research proposals for funding agencies;
Have provided external reviews of more than 30 tenure and promotion cases at research universities in North America

Awards and Honors

2018 *Member, EU Academy of Sciences*
2015 *Excellent Service Award, International Association for China Planning (IACP)*
2013 *Jammal Fellow, University of Buffalo*
2011 *Best Paper Award, World Society of Transportation and Land Use Researchers (WSTLUR) (for paper co-authored with Lei Zhang, Jin Hyun Hong, and Arefeh Nasri)*

2010 *Chester Rapkin Award, Association of Collegiate Schools of Planning (ACSP) (for journal article co-authored with Joseph Grengs, Jonathan Levine, and Qingyun Shen)*
1999 *Mitsui Career Development Chair (3 year re-appointment), MIT*
1999 *Emerging Scholar Paper Award, Spatial Analysis and Modeling Specialty, Association of American Geographers (AAG)*
1998 *Horwood Critique Prize, Urban and Regional Information Systems Association (URISA)*
1996 *Mitsui Career Development Chair (3 year appointment), MIT*

Urban spatial structure refers to not only the spatial arrangement of, but more fundamentally also the functional relations between, the socioeconomic activities in a city or metropolitan region. These functional relations are established through transportation (and increasingly, remote communication), and in turn generate the intra-city or intra-metropolitan movement of people, material goods, and information. Understanding this interactive, and increasingly dynamic and complex, relationship between urban spatial structure and transportation is essential for planning and policymaking aimed at creating economically productive, socially equitable, and environmentally sustainable cities. The following sections present a brief summary of my past accomplishments and current projects in this research field.

Measurement and Analysis of Urban Spatial Structure

The most important component of my research has been to develop accessibility measures for the analysis of urban spatial structure. Economists, including most notably, Alonso (1964), traditionally used a highly simplified measure of accessibility—the distance from market place or city center—and its tradeoffs with bid-rent for land to derive an equilibrium model of urban spatial structure and land use. While this approach resulted in a powerful conceptual framework, it did not offer a practical measure that indicates the ease of reaching destinations that are typically distributed in different parts of a city. Consequently, a number of accessibility measures were developed as analytical tools for examining urban spatial structure and informing urban planning. The gravity formulation proposed by Hansen (1959), which quantifies accessibility as the sum of relevant opportunities weighted by spatial impedance, has been the most widely applied measure.

I have modified the Hansen accessibility measure to make it suitable for contexts where the opportunities are rival goods and hence the spatial distribution of competitions must be considered (Shen, 1998a). The measure I have developed is a generalized form of the formula appeared earlier in Weibull (1976), and it incorporates any number of alternative travel modes and has trackable statistical properties. This accessibility measure is especially useful for analyzing the spatial structure of metropolitan labor market, where job seekers who use different transportation modes for daily travel compete for limited number of job openings. Empirical studies applying this measure have clearly shown the critical role of transportation in determining employment accessibility in contemporary metropolitan areas characterized by spatial dispersion of economic opportunities (Shen, 1998a; Shen, 2001). Transit-dependent low-income workers are at a distinctive spatial disadvantage in competing for economic opportunities, even if they live in central areas with some location advantage (Shen, 1998a; Kawabata and Shen, 2007).

I have extended the accessibility framework in light of the transformation of urban spatial structure driven by information and communication technologies (ICT) (Shen, 1998b; Shen, 1999; Shen, 2000b). Today, economic opportunities exist not only in physical space, but also increasingly in virtual space (accessible only remotely through ICT, such as the internet and mobile phone) and hybrid space (accessible either remotely

through ICT or physically through transportation). A unified accessibility measure is constructed by spatially and temporally connecting activities in physical and virtual spaces, and by embedding the latter in the former for the purpose of quantifying spatial impedance (Shen, 2000b; Shen, 2003). For example, a worker's telecommuting days can be linked to the remaining workdays when she commutes to workplace, and her daily average commuting time and spatial impedance can be estimated. Not surprisingly, ICT have substantially widened accessibility gaps among population groups, with low-income workers finding themselves in an increasingly disadvantaged position.

My other noteworthy past research in this area examined the role of government policy—in the forms of municipal growth controls and state smart growth initiatives—in shaping urban spatial structure. My empirical studies focused on the effects of these policies on the intra-metropolitan distribution of urban growth (Shen, 1996; Shen and Zhang, 2007). The studies employed statistical models of urban growth for both pre- and post-policy periods to help assess the effects. Based on data from California and Maryland, the government policies were shown to have created significant impacts on the region-wide spatial patterns of urban development.

Currently, I am working with several colleagues to gain a deeper understanding of mixed land use as an important characteristic of urban spatial structure. Starting with the observation that mixed land use is commonly observed in cities but not satisfactorily explained by existing neoclassical economic theories, we are exploring alternative theoretical frameworks to help conceptualize mixed land use and guide its evaluation (Shen and Sun, 2017). In particular, we are drawing from the transaction cost economic theory (Williamson, 1985) in our research effort, which aims to use real estate data and land use data to examine the underlying mechanisms of mixed use development and assess its economic benefits under various conditions.

Effects of Urban Spatial Structure on Transportation and other Outcomes

Another major part of my research has focused on the effects of urban spatial structure, measured by accessibility indices or built environment characteristics, on transportation and urban sustainability outcomes. Several of my empirical studies have demonstrated that urban spatial structure is a powerful explanatory factor of workers' commuting duration, and that its influence on transit riders is especially significant (Shen, 2000a; Shen 2003; Kawabata and Shen, 2007). The impact of urban spatial structure on low-income workers' employment status is much more complicated, as panel data on housing location and automobile ownership for welfare recipients in an American city has shown (Shen and Sanchez, 2005). To increase their likelihood to find employment, these low-income workers tended to relocate to neighborhoods with less poverty and more racial integration rather than to neighborhoods with higher accessibility, while buying a car as a way to increase transportation mobility.

My research explored how ICT may enlarge the geographic extent of urban spatial structure by reducing workers' commuting frequency and increasing workers' residential location flexibility, and how this may generate a secondary effect on transportation outcome in the form of longer trips (Shen, 2000c). Thus the direct partial-substitution of ICT for travel is likely to be combined with indirect generation of extra travel distances, leaving the overall outcome uncertain. Again, the impact is differentiated between people who travel by private automobile and people who rely on public transportation, as the location flexibility of the latter is still largely constrained by the geographic coverage of public transportation service.

I have worked with colleagues in exploring new methodological approaches for uncovering the complex relationships between built environment characteristics and transportation outcomes. In one study, we reexamined the built environment-travel behavior relationship by addressing several commonly observed methodological issues simultaneously (Hong, Shen, and Zhang, 2014). The results indicated that land use factors have highly significant effects on vehicle miles traveled (VMT) even after controlling for the attitudinal factor and spatial autocorrelation. In another study, we estimated structural equation models (SEMs) to examine how the built environment affects transportation fuel consumption (Liu and Shen, 2011). We found that the built environment creates an indirect effect on fuel consumption through influencing the vehicle type, travel mode choice, and driving speed. In a third study, my colleagues and I employed naturalistic driving data to examine the impacts of the built environment on vehicle fuel consumption rate (Wang, Liu, Kostyniuk, Shen, and Bao, 2014). Results of our SEMs showed that some common features of compact urban development, including high intersection density and higher employment density, are associated with lower driving speed, more speed changes, and lower fuel efficiency. In other words, while compact development generally encourages shorter trips and greater shares of non-motorized modes, it may also result in higher fuel consumption per unit of driving distance.

I have also researched on the connection between urban spatial structure and transportation in China. In the mid-1990s, large Chinese cities were experiencing dramatic urban spatial transformation resulting from market-oriented economic reforms; they were also at the early stage of rapid motorization enabled by rapid economic growth. Observing that travel demand in Shanghai was increasing explosively through a combination of more trips, longer trips, and mode shifts from walk and transit to the automobile, I proposed that physical planning together with complementary policies should be employed to effectively address transportation issues (Shen, 1997). About 15 years ago, after two decades of fast-paced motorization, large Chinese cities started to see rail transit as the key to counter growing automobile dependence. My colleagues and I recently examined the effectiveness of building an extensive rail transit system to support urban growth in Shanghai (Shen, Chen, and Pan, 2016). Our results showed that this strategy increases the likelihood of choosing rail transit for commuting, especially the long-distance trips, but does not seem to directly influence car ownership. On the other hand, the results also suggested that considerations of money, time, comfort, and safety exert measurable influences on both mode choice and car ownership, and that the intention to ride the metro for commuting is reflected in its actual use as primary mode for journey to work.

Currently I am working with several colleagues to gather empirical evidence on the travel behavior impacts of mobile technologies-supported shared mobility services. We are interested in gaining an understanding of how ride-hailing and car-sharing services affect the mode choice, VMT, and car ownership of geographically and economically differentiated population groups, as well as their patterns of substitution and/or complementarity with public transportation and non-motorized travel. We are also interested in exploring innovative travel demand management ideas and policies that work for this new era. An overarching question is: Can collaboration between public and private mobility services be established, such that it improves the overall efficiency of the transportation system while safeguarding the accessibility needs of disadvantaged groups?

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Contributions in Cardiovascular Prevention & Hypertension

by Giuseppe Mancia, Member EUAS

Short Biography

PRESENT POSITION. *GM is Professor Emeritus of the University Milano.-Bicocca. He is also Head of the Hypertension Center, university Institute, Verano, Policlinico di Monza, President of the Italian Foundation on "Ricerca e Innovazione su Ipertensione e Protezione Cardiovascolare" and Chairman of the Foundation of the European Society of Hypertension (ESH, Zurig). He serves since 2008 as Chairman of the Joint Board of the Italian Scientific Societies operating in the area of cardiovascular prevention.*

DEGREES/DIPLOMAS. *He trained at the University of Siena, Medical School, where he graduated in 1964 cum laude. He obtained in 1967 the Post-graduate Diploma (cum laude) of Specialist in Cardiology and Rheumatology while working as an investigator of the National Research Council. He obtained the Ph.D. (Libera Docenza) in Physiology in 1970 and worked as Post-graduate Fellow of the US Public Health Service and Associate Researcher at the Mayo Clinic (1972-1974).He has then been Resident in the Postgraduate School of Cardiology of the Virginia Commonwealth University(1974)*

ACADEMIC/HOSPITAL POSITIONS. *GM has been Assistant and Associate Professor of Internal Medicine at the University of Milan from 1969 to 1985.From 1985 he has been appointed full Professor of Internal Medicine at the University of Milano first and Milano-Bicocca later. From 1992 he has been Head of the Division of Internal Medicine and Chairman of the University and Hospital Departments of Clinical Medicine (S. Gerardo Hospital, Monza).He has also been Director of several Postgraduate Schools of Medicine (Cardiology, Internal Medicine, Emergency Medicine and Endocrinology),University Masters (Transplant Medicine, Electrophysiology and Cardiac Electro-Stimulation),and the Research Doctorate in Hypertension and Cardiovascular Risk. He has chaired the Interuniversity (Universities of Milano, Milano-Bicocca and Pavia) Center of Clinical Physiology and Hypertension from 2001 to 2012 .*

SCIENTIFIC SOCIETES/TASK FORCES/COMMITTEES. *GM has served as President (1988-1990) of the International Society of Hypertension (ISH), President of the European Society of Clinical Investigation (1980-1982), Chairman of the Working Group on Hypertension and the Heart of the European Society of Cardiology (ESC,1994-1996), member of the Executive Scientific Committee of ESC (1986-1991), President of the Italian Society of Hypertension (1997-1999) and President of ESH (1999-2001). He has been member ex-officio (only European) of the Executive Council of the American Society of Hypertension (1996-2008), Officer for the ISH Forum of National Societies, member of the Committee on Cardiovascular Drugs and Therapy of the World Heart Federation and member of the Writing Committee of the ESC guidelines on Prevention of Cardiovascular Diseases (1993, 1998, 2003),the WHO/ISH Guidelines on Hypertension (1993, 1999) and the Guidelines on Hypertension in the Elderly of the American College of Cardiology (2011,only European).He has co-chaired the Task Force on the ESH-ESC guidelines on Hypertension (2003,2007,2009 and 2013 and 2018), the WHO/ISH Liaison Committee, and the Scientific and Organising Committees of various ESH Meetings (2001, 2003, 2005, 2007, 2009, 2011, 2013,2015,2017). He has been Chairman of the Scientific Committee of the ISH Congress in Prague (2002) and Honorary President of the ISH Meeting in Montreal (1990),the ISH Meeting in San Paulo (2004), and the ESH/ISH Meeting in Athens (2014).He is currently Chairman of the Educational Board of ESH.*

AWARDS/HONORS.*GM has received several Awards, among which the Heymans Award of the International Society of Pharmacology, the Wright International Award of the High Blood Pressure Council of Australia, the ISH Volhard and the Tigersted (MSD) Awards, the ESH Folkow Award and the Life Achievement Award of the Italian Society of Hypertension. He was appointed Lecturer of the Year by the Belgian Universities and Hypertension Leagues (1992) and was conferred the Talal Zein Foundation Award, the International Recordati Prize (2000), the 2001 Invernizzi Award for Medicine, the Gold Medal of the Lorenzini Foundation (2008),the Hariri Memorial Award (2009) and the Spinoza Award of the Amsterdam University.He has been appointed Honorary Member of ESH, the High Blood Pressure Council of Australia, the Latino-american Hypertension Society(LASH) and the Japanese Circulation Society. He is honorary member of many other Scientific Academies or Societies, among which the British Hypertension Society, the German Hypertension League ,the Spanish Hypertension Society, and the Hellenic Cardiology Society . He has received the highest Award of the Lombardy Region (Rosa Camuna) and the title of Commander of the Order of the Italian Republic in 2014.He has recently been awarded as one of the 100 italian excellences in various areas of human activities (Award ceremony in the Italian Parliament ,December 2015).He is member of the 2003 Group for Research (the Group of the Italian scientists most highly cited in the world) and member of the European Academy of Sciences*

He has been invited to give state-of-the-art, keynote, debates or special and plenary lectures in more than 700 international meetings. He has also been guest lecturer at meetings of many national societies of hypertension,

cardiology awarded as one and internal medicine, among which the Pickering Lecture (British Hypertension Society), the Tigersted Lecture (Finnish Hypertension Society), the Merck Frosst Lecture (Canadian Society of Cardiology), the Saeb Salam Memorial Lecture (Beirut University), the Brian Bronte Steward Memorial Lecture (Glasgow University) the Leloir Nobel Laureate Lecture (Buenos Aires),the Mac Donald Lecture (Hamilton),the Gavras Life Achievement Award Lecture (Athens),and the Population Health Lecture (Mac Master University,Hamilton).

***HONORARY DEGREES/ACADEMIC RECOGNITIONS**.GM has received the Honorary Professorship of the University of Cordoba. He is Honorary member of the Academy of Science of Cordoba, and has been conferred the Degree Honoris Causa in Medicine from the University of Gdansk and the Carol Davila University of Bucharest. He has also received the Degree Honoris Causa (Doctor of Science) from the University of Glasgow..*

***EDITORIAL ACTIVITY**. GM has edited more than 90 Special issues or Supplements to international cardiovascular and internal medicine Journals. He has written or edited more than 20 books on hypertension, metabolic diseases and cardiovascular diseases edited by international Publishers, among which several Manuals, including the official one of ESH. He is or has been member of the Editorial Board and Reviewer of the most important international journal on hypertension cardiovascular disease and internal medicine. He is Chief-Editor of the official ISH/ESH Journal (Journal of Hypertension)*

***SCIENTIFIC ACTIVITY**. GM's research interests focus on epidemiology pathophysiology, diagnosis and treatment of hypertension, heart failure, and coronary disease, as well as on the clinical aspects of diabetes, obesity and other metabolic abnormalities. His expertise includes ambulatory blood pressure monitoring, neurohumoral control of the circulation, large artery mechanics, hemodynamic changes of cardiovascular drugs, cardiovascular regulation during stress and sleep as well as epidemiology and intervention trials in hypertension and diabetes. He has been member or chairman of the steering committees of several clinical trials. He has published more than 2000 original papers, reviews and editorials in peer-review journals. One of his papers has been the most highly cited article in the world medical literature during 2004-2005 (Ref. The Scientist) and three have been included among the most widely quoted hypertension papers ever (Ref. Hypertension,2014).He is since many years in the list of the "highly cited" scientists (Thompson Reuters and Clarivate Analytics) and has in 2013 been regarded as one of the 400 most influential biomedical investigators in the world (EJCI). GM's publications have received, up to December 2018, almost 200.000 citations in the international medical literature, with a H-index For the 1982-2018 papers of 162(Ref Microsoft Academy),the highest among Italian internists and cardiologists.*

Sympathetic Nerve Traffic Activation in Essential Hypertension and Its Correlates Systematic Reviews and Meta-Analyses

Guido Grassi, Anna Pisano, Davide Bolignano, Gino Seravalle, Graziella D'Arrigo, Fosca Quarti-Trevano, Francesca Mallamaci, Carmine Zoccali, ***Giuseppe Mancia***

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Muscle sympathetic nerve activity (MSNA) has shown that sympathetic activation may occur in essential hypertension (EHT). However, the small sample size of the studies, the heterogeneity of the patients examined, and the presence of confounders represented major weaknesses not allowing to draw definite conclusions. Among the 432 studies identified providing information in EHT on MSNA, 63 were eligible (1216 patients) and metaanalyzed grouping them on the basis of clinically relevant questions: (1) Is MSNA increased in hypertension of mild/moderate-to-severe degree? (2) Does sympathetic activation occur in borderline, white-coat, and masked EHT? (3) Is MSNA related to clinic and ambulatory blood pressure and target organ damage? (4) Are heart rate and venous plasma norepinephrine valuable surrogate markers of MSNA in clinical practice? The results show that MSNA was significantly greater (1.5×; $P<0.001$) in mild-to-moderate and severe EHT as compared with normotensive controls and that this was the case also in borderline, white-coat, and masked hypertension as well. Interestingly, MSNA was significantly greater in both untreated and treated hypertension ($P<0.001$ for both), related to clinic and ambulatory blood pressure ($r=0.67$ and $r=0.83$; $P<0.001$ for both), inversely related to heart rate ($r=-0.38$; $P<0.001$) and directly to venous plasma norepinephrine ($r=0.28$; $P<0.001$) and left ventricular mass index ($r=0.27$; $P<0.001$). Thus, EHT is a

condition characterized by a sustained sympathetic overdrive, whose magnitude is proportional to its clinical severity. This is more clearly manifest when MSNA rather than indirect markers of adrenergic drive, such as heart rate and plasma norepinephrine, are used.

Global Impact of the 2017 American College of Cardiology/American Heart Association Hypertension Guidelines.
A Perspective From Italy

***Giuseppe Mancia**, Giovanni Corrao*

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The 2017 American College of Cardiology/American Heart Association (ACC/AHA) hypertension guidelines have several important elements of novelty, and some weaknesses, as well. One strength is that, unlike the most recent US hypertension guidelines (the Joint National Commission 8 guidelines), the ACC/AHA document does not cover only a few items, eg, blood pressure (BP) threshold and target for treatment, but rather it deals with multiple aspects of hypertension diagnosis and treatment that, although unaddressed or nonaddressable by randomized clinical trials, have major importance for clinical practice. Another is that each issue is synthetically and clearly discussed in terms of its scientific evidence (thereby fulfilling the guidelines' educational role) while still providing simple conclusions and recommendations according to a format that resembles the one used in the European Society of Hypertension/European Society of Cardiology guidelines. However, the new guidelines discuss the available evidence in a manner that is more complete than that used by the European and other guidelines, because it includes the level and strength of evidence for a given intervention, separating those which do not provide benefits from those which may cause harm.

The ACC/AHA guidelines take a strong position in favor of 3 major changes in antihypertensive treatment strategies, in line with the evidence from new randomized outcomes trials or comprehensive meta-analyses. One, the need for drug treatment to be extended to all individuals with a BP ≥140/90 mm Hg is proposed, independent of age and cardiovascular risk level, at variance from previous recommendations to use antihypertensive drugs cautiously in grade 1 hypertension in patients at low to moderate risk and to pharmacologically treat older patients only if their systolic BP is closer to or >160 mm Hg. Two, it is recommended to reduce BP to values lower than those previously recommended for the general and older population, in agreement with the results of both the SPRINT trial (Systolic Blood Pressure Intervention Trial)3 and several large meta-analyses that have shown that a systolic BP reduction to <130 mm Hg may afford incremental benefit. Three, a recommendation to start treatment with 2 rather than 1 drug in patients with a BP ≥140/90 mm Hg is proposed, a strategy never recommended on such a general basis by previous US guidelines and considered in the European guidelines only for patients at high cardiovascular risk, based on the possibility that the more rapid BP reduction that accompanies an initial 2-drug regimen might provide added protection. It should be noted that this novel ACC/AHA recommendation does not stem from the results of a randomized outcomes trial, because no trial has compared cardiovascular risk in patients starting treatment with 2 drugs versus those starting with 1 drug and moving to a combination later. It is, however, supported by the finding that, in clinical practice, initial

combination treatment is associated with better long-term BP control and, observationally, a lower risk of cardiovascular events. This may be accounted for by improved long-term adherence to a combination treatment regimen in light of the failure of patients on initial monotherapy to move to administration of ≥2 drugs when BP control is inadequate, a phenomenon known as therapeutic inertia. Initial combination treatment may thus mitigate factors involved in the worldwide poor rate of hypertension control, favoring its improvement after decades in which control has shown either no change or a small increase in some countries.

The ACC/AHA guidelines have some weaknesses as well. For example, these guidelines devote little attention to asymptomatic organ damage such as left ventricular hypertrophy or increased urinary protein excretion whose detection may more precisely quantify cardiovascular risk and perhaps patient protection with treatment, as well. We are also not enthusiastic about the way the classification of BP values issued in the 2003 Joint National Commission guidelines has been modified. Whereas the ACC/AHA guidelines now recommend drug treatment in a large fraction of patients with a high-normal BP (those with a 10-year risk of a cardiovascular event >10%), there was probably no need to rename this BP range as grade 1 hypertension. There was also no need, in our opinion, to consider individuals with a systolic BP between 120 and 129 mm Hg as having BP elevation, a definition that may substantially increase the number of subjects categorized with BP abnormality, especially in the elderly. On the basis of data from the PAMELA study (Pressioni Arteriose Monitorate E Loro Associazioni) (age range, 25–74 years; mean, 50.9±13.7) in Italy, ≈22% of the population previously defined as having a normal BP would now migrate to a BP elevation range. In addition, a substantial fraction of subjects previously included in the high-normal BP range (≈17% of the population) would now be flatly termed hypertensive, requiring pharmacological or lifestyle intervention. We also wonder about the feasibility and usefulness of the ACC/AHA recommendations to detect white coat or masked hypertension by measuring out-of-office BPs any time office systolic BP is between 120 and 159 mm Hg, because (1) this range includes a huge number of individuals, and (2) in either condition the effects of treatment are unknown, and thus detection does not translate into evidence-based therapeutic action. The new guidelines set the systolic BP goal at <130 mm Hg in the entire hypertensive population, rather than at <140 or 150 mm Hg as in previous guidelines, which has the merit of simplifying the treatment goal and avoiding confusion. This change, however, affords little consideration of the fact that (1) the association of this lower target with enhanced protective effect is weak or absent in several clinically important patient subgroups, including the elderly, and (2) lower BP goals are accompanied by a marked increase in serious side effects, ie, a major cause of treatment discontinuation that is followed by a pronounced increase in cardiovascular risk. This might argue in favor of a more conservative position, at least in older patients in whom BP-related side effects are more common. That being said, and regardless of any possible criticism, the ACC/AHA guidelines represent an important document that may promote change in a more effective direction for the management of hypertension. If more extensively adopted in clinical practice, initial 2-drug combination treatment may meaningfully increase hypertension control in the population, thereby addressing a devastating phenomenon that maintains hypertension as the leading cause of death worldwide.

Blood pressure targets in type 2 diabetes. Evidence against or in favour of an aggressive approach

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When associated with high blood pressure, type 2 diabetes mellitus is characterised by a high risk of adverse cardiovascular (CV) and renal outcomes. However, both can be effectively reduced by antihypertensive treatment. Current guidelines on the treatment of hypertension emphasize the need to effectively treat high blood pressure in diabetic individuals, but their recommendations differ in terms of the optimal target blood pressure value to aim for in order to maximise CV and renal protection. In some guidelines the recommended target blood pressure values are <140/90 mmHg (systolic/diastolic), whereas in others, blood pressure values close or even less than 130/80 mmHg are recommended. This paper will discuss the evidence for and against a conservative or more aggressive blood pressure target for treated diabetic hypertensive individuals based on the evidence provided by randomised trials, trial meta-analyses and large observational studies. Based on the available evidence, it appears that blood pressure targets will probably have to be lower than <140/90mmHg, and that values approaching 130/80mmHg should be recommended. However, evidence in favour of even lower systolic values, i.e. <130 mmHg, is limited and is definitively against a reduction to <120 mmHg.

Initial Antihypertensive Treatment Strategies and Therapeutic Inertia
Evidence From a Large Population-Based Cohort

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In many hypertensive patients, treatment is not upgraded despite lack of blood pressure control because of therapeutic inertia. Information is limited, however, on the extent of this phenomenon in real-life medicine. We studied 125 635 patients (age 40–85 years) from the Lombardy region (Italy) who started antihypertensive treatment with 1 drug (n=100 982) or a 2-drug fixed-dose or free combination (n=24 653). A log-binomial regression model was used to estimate the prevalence ratio of combination therapy in relation to the initial treatment strategy. In the initial monotherapy group, patients under drug combinations were 22%, 27%, 32%, and 36% at 6 months, 1, 2, and 3 years later. In the initial combination treatment group, the corresponding percentages were 85%, 82%, 79%, and 78%. This translated into a markedly greater covariate-adjusted propensity of being under a multidrug prescription throughout the follow-up: 3.92 (95% CI, 3.84–4.00) after 6 months and 3.18 (3.12–3.25), 2.56 (2.51–2.60), and 2.23 (2.19–2.27) after 1, 2 and 3 years of treatment. In a propensity score analysis, initial 2-drug combination treatment was also associated with significant reductions in the risk of death (−20%, 11% to 28%) and hospitalization for cardiovascular events (−16%, 10% to 21%) compared with initial monotherapy. Thus, in real life, a large number of patients prescribed initial monotherapy fails to move to combination treatment, as recommended by guidelines. This implies that therapeutic inertia frequently prevents proper treatment uptitration, thereby playing a major role in the low rate of hypertension control that exists worldwide.

New Modified Embedded Atom Method (MEAM) Potential including the Bond Order (MEAM-BO) to describe the Energetics of Unsaturated Hydrocarbons

by Mark F. Horstemeyer, Member EUAS

Short Biography

Mark F. Horstemeyer, Dean of Engineering, Liberty University

As a fellow of four societies (ASME, ASM, SAE, and AAAS) Dr. Mark F. Horstemeyer has published close to 500 journal articles, conference papers, books, and technical reports with a citation impact h-factor over 60 with a total of over 12,000 citations; he has been invited to give over 150 lectures throughout the world (was named as honorary professor of Xihua University, Chengdu, China); and has won many awards (R&D 100 Award, AFS Best Paper Award, Sandia Award for Excellence, Ralph E. Powe Research Award, Ohio State's Thomas French Alumni Achievement Award); and has mentored over 120 graduate students and post-doctoral researchers. He has started two start-up companies in trying to put predictive science into engineering designs: Predictive Design Technologies, LLC; Advanced Technology Associates, LLC. He earned a B.S. degree (with honors) from West Virginia University in Mechanical Engineering in 1985, a M.S. degree from Ohio State University in Eng. Mechanics in 1987, and a Ph.D. from Georgia Institute of Technology in Mech. Eng. and Math & Matls (minors) in 1995. He is currently Dean of Engineering at Liberty University. Previous to that, he worked at Sandia National Labs (1987-2002) and Mississippi State University (2002-2018), where he held a Chair position for the Center for Advanced Vehicular Systems (CAVS) in Computational Solid Mechanics. He couples multidiscale, multiphysics research of mechanics and materials in three synergistic areas: theoretical modeling, experimentation, and large scale parallel computational simulation.

A new Modified Embedded Atom Method (MEAM) potential that includes the bond order (MEAM-BO) to describe the energetics of unsaturated hydrocarbons (double and triple carbon bonds) was developed. Such quantities like bond lengths, bond angles, and atomization energies at 0 K,

dimer molecule interactions, rotational barriers, and the pressure–volume-temperature relationships of dense systems of small molecules give a comparable or more accurate property relative to experimental and first-principles data than the classical reactive force fields REBO and ReaxFF.

Our extension of the MEAM potential for unsaturated hydrocarbons (MEAM-BO) is a step toward developing more reliable and accurate polymer simulations with their associated structure–property relationships, such as reactive multicomponent (organic/metal) systems, polymer–metal interfaces, and nanocomposites. When the constants for the BO are zero, MEAM-BO reduces to the original MEAM potential. As such, this MEAM-BO potential describing the interaction of organic materials with metals within the same MEAM formalism is a significant advancement for computational materials science.

Regarding MEAM-BO, to correctly model the interaction between molecules, dispersion forces have been included via the DFT-D3 modification. It is demonstrated that this semi-empirical classical potential correctly reproduces the behavior of the S2 dimer, various cyclic sulfur rings, the molecular solids α-, β-, and γ-sulfur, and a number of theoretical, high symmetry sulfur structures. This potential will serve as a useful tool in the atomistic modeling of sulfur and, ultimately, in the modeling of sulfur containing organic compounds using this updated MEAM-BO formalism.

MEAM-BO was used on a biological material system used to provide information for continuum finite element material models. One mechanism related to traumatic brain injury is membrane mechanoporation, which can occur during physical insults and can be devastating to cells, depending on the level of disruption. The current study investigates the strain state dependence of phospholipid bilayer mechanoporation and failure. Using molecular dynamics, a simplified membrane, consisting of 72 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) phospholipids, was subjected to equibiaxial, 2:1 non-equibiaxial, 4:1 non-equibiaxial, strip biaxial, and uniaxial tensile deformations at a von Mises strain rate of $5.45 \times 10^8\ s^{-1}$, resulting in velocities in the range of 1 to 4.6 $m \cdot s^{-1}$.

A water bridge forming through both phospholipid bilayer leaflets was used to determine structural failure. The stress magnitude, failure strain, headgroup clustering, and damage responses were found to be strain state-dependent. The strain state order of detrimentality in descending order was equibiaxial, 2:1 non-equibiaxial, 4:1 non-equibiaxial, strip biaxial, and uniaxial. The phospholipid bilayer failed at von Mises strains of .46, .47, .53,

.77, and 1.67 during these respective strain path simulations. Additionally, a Membrane Failure Limit Diagram (MFLD) was created using the pore nucleation, growth, and failure strains to demonstrate safe and unsafe membrane deformation regions. This MFLD allowed representative equations to be derived to predict membrane failure from in-plane strains.

These results provide the basis to implement a more accurate mechano-physiological internal state variable continuum model that captures lower length scale damage and will aid in developing higher fidelity injury models.

Contributions in Membrane Science & Engineering

by Enrico Drioli, Member EUAS

Short Biography

Prof Enrico Drioli

Emeritus Professor, University of Calabria

CAREER

Distinguished Visiting Professor at Nanjing Tech Univesity, College of Chemical Engineering (2018 - ~)

Guest Professor of School of Marine Science and Technology of Harbin Institute of Technology, Weihai, P.R.China (01 January 2018 – 31 December 2020)

Distinguished Visiting Professor, Faculty of Engineering & Information Technology, University of Technology Sydney, Australia (January 2016)

BrainKorea21 Program (BK21 Plus) Distinguished Visiting Professor, Department of Energy Engineering, Hanyang University, Seoul Korea (2016-present)

Visiting Professor at Nanjing Tech University. Membrane Center (November 2014 – 2016- 2017)

Distinguished Adjunct Professor, Center of Excellence in Desalination Technology, King Abdulaziz University, Jeddah Saudi Arabia (2012)

WCU (World Class University) Distinguished Visiting Professor, Department of Energy Engineering, Hanyang University, Seoul Korea (2009)

Emeritus Professor, School of Engineering of the University of Calabria (2012)

Professor of Chemistry and Electrochemistry at the School of Engineering of the University of Naples (since 1968-1982)

Professor at the School of Engineering of the University of Calabria (1981-2011).

Dean of the School of Engineering of the University of Calabria (1982-1985).

Founding Director of the Institute on Membrane Technology (ITM) of CNR (from 2011)

Director of the Institute on Membranes and Chemical Reactors of the National Research Council (1993 - 2001).

Director of the Institute on Membrane Technology (ITM) of CNR (2002 - 2008)

RESEARCH INTEREST

Membranes in Artificial Organs, Integrated Membrane Processes, Membrane Preparation Transport Phenomena, Membrane Distillation and Membrane Contactors, Catalytic Membrane and Catalytic Membrane Reactors

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Coordinator of the European Erasmus Mundus Doctorate in Membrane Engineering (EUDIME);

Scientific Coordinator of various international Contracts/Agreements: ITM-CNR-KACST - (1)Hydrophobic membrane preparation for membrane contactors application; ITM-CNR-KISR (Kuwait Institute for Scientific Research) - Evaluation of the potentialities of the membrane distillation technology for desalting de-oiled filtered high concentrated saline waters; RHODIA; etc

Member of the Scientific Advisory Panel (SAP) for the KAUST Water Desalination and Reuse (WDR) Center from 2010; Coordinator or Scientific responsible in various EU projects: MATChING - Materials &Technologies for Performance Improvements of Cooling Systems in Power Plants ; IDEA - Development of a solar powered, zero liquid discharge Integrated DEsalination MembrAne system to address the needs for water of the Mediterranean region ; NAWADES - NAnotechnological application in WAter DESalinitation; CapWa - Capture of evaporated water with novel membranes; Membrane- Based Desalination: an

Integrated Approach acronym MEDINA; ect.;
Lifetime Achievements Awards in the cause of membrane separation in China, Qingdao Int. Water congress Selective Committee, China (June 2017), Ambassador of Friendship Certificate of Shandong Province in "acknowledgement of his contribution to the Province", China (2017), Honorary Citizen Weihai City, China, for his contribution to Weihai City development (2016), Award with the Academician Semenov Medal of Russian Academy of Engineering Science (2014)
Honorary Membership of the Czech Society of Chemical Engineering (2012)
2011, "Richard Maling Barrer Prize" of the EMS, for his "outstanding contributions to membrane science and technology"
2009, Doctorate Honoris Causa from University of Paul Sabatier of Toulouse, France
2005, International Cooperation Honor Award, Membrane Industry Association of China (MIAC) for special dedication to International Cooperation between China and Europe in the field of membrane science and technology
2005 – Present, Guest professor, Jiangsu Polytechnic University, China
1999, Honorary President, European Membrane Society
1992, Doctorate Honoris Causa in Chemistry and Chemical Technology, Russian Academy of Science
1991, Honorary Professor, China Northwest University in Xi'an, Shaanxi, China
1982 – 1998, President, European Society of Membrane Science and Technology (European Membrane Society)
Advisory Board of "Journal of Membrane Science", of "Polish Journal of Chemical Technology"; Editorial Board of various other international scientific Journals.
Exec. Editor: Applied Water Science Journal, Springer Berlin Heidelberg (Germany) and Membrane Water Technology, Techno Press (Korea)
Author of more of 880 scientific papers, 22 patents, and 29 books

L. Donato, M. R. Gullo, O. I. Parisi, E. Drioli, C. Algieri, F. Puoci, Development of novel hybrid imprinted membranes for selective recovery of Theophylline, Separation and Purification Technology (192, pp. 513-519), 2018.

Abstract

A theophylline-binding polymer was synthesized utilizing the bulk polymerization technique. Methacrylic acid, ethylene glycol dimethacrylate, 2,2′-azoisobutyronitrile and chloroform were used to synthesize the imprinted polymer. Theophylline was employed as template. The obtained polymer powder were dispersed in the modified poly(ether ether ketone) (PEEK-WC) polymer solution for preparing hybrid imprinted membranes via the phase inversion technique. Membranes containing the non-imprinted polymer were also prepared and used as reference. For evaluating the recognition properties of polymers and membranes re-binding experiments, with the template and its structural homologue caffeine, were carried out. The binding capacity of MIP towards the template was 1.18 μmol/gp and the theophylline/caffeine selectivity factor was 3.2. All the imprinted membranes exhibited good recognition properties compared with blank membranes, which only showed a poor non-specific binding.The membrane containing 30 wt% of the imprinted polymer exhibited the highest binding capacity (10.97 μmol/gmemb.), and a theophylline/caffeine selectivity factor of 71.42.

Ali, A., Tsai, J.-H., Tung, K.-L., Drioli, E., Macedonio, F., Designing and optimization of continuous direct contact membrane distillation process, Desalination 426, pp. 97-107, 2018.

Abstract

Membrane distillation (MD) is a relatively less-explored membrane operation with the potential to achieve high recovery factor by using low grade heat. The current study proposes the design of a continuous direct contact MD process to achieve high recovery factors by using a commercial hollow fiber membrane. The design consists of multiple MD stages connected in series to achieve a predefined final solution concentration. Depending upon the outlet temperatures of feed and permeate, the design considers the option of heat recovery from permeate. Under a given set of operating conditions, there exists a module length (named as optimum module length) where the net thermal energy consumption and overall permeate productivity are optimum. The optimum

module length has been analyzed as function of feed to permeate flow rate (F/P) ratio, feed temperature and concentration. It has been observed that for given feed temperature and concentration, the optimum module length can be tuned by changing F/P ratio. The minimum value of the optimum length is observed at the highest F/P ratio considered. Mathematical analysis was extended to evaluate the appropriate length and the corresponding thickness for each stage. The results reveal a strong nexus among membrane thickness, solution concentration and optimum length.

Ali, A., Tufa, R.A., Macedonio, F., Curcio, E., Drioli, E., Membrane technology in renewable-energy-driven desalination, Renewable and Sustainable Energy Reviews 81, pp. 1-21, 2018.

Abstract

Growing requirements of freshwater and unsustainable nature of fossil fuels are driving the interest in using renewable energy for desalination applications. Due to their less energy-intensive nature and small footprint, membrane-based desalination operations are gaining significant interest in this regard. Substantial efforts have been observed in integrating traditional renewable and relatively green sources of energy (wind, solar, geothermal, tidal and nuclear) with membrane-based desalination operations, mainly reverse osmosis (RO) and electrodialysis (ED). Due to recent developments and progresses in membrane technology, interesting membrane operations including membrane distillation (MD), pressure retarded osmosis (PRO) and reverse electrodialysis (RED) have emerged. These operations are capable of generating clean and sustainable electricity from various waste streams including brine and impaired water which otherwise are considered environmental liabilities. PRO and RED require mixing of a high salinity solution (such as seawater or brine and wastewater, respectively) with a low salinity solution to generate electricity. MD has shown the potential to generate freshwater and electricity as standalone process. Integration of MD with PRO or RED enhances the performance of these processes and provides a clean and sustainable route to produce freshwater and energy. The current study reviews the recent progresses and developments in applying renewable energy sources in membrane based desalination with special attention on emerging membrane operations with proven capability to generate energy from wastewater streams.

Z.Cui., Y. Zhang, X. Li, Xi. Wang, E.Drioli, Z. Wanga, S.Zhao, Optimization of novel composite membranes for water and mineral recovery by vacuum membrane distillation, Desalination, Volume 440, 15 August 2018, Pages 39-47.

Abstract

In mining industries, the process combining ultrafiltration (UF) and reverse osmosis (RO) is often used for wastewater treatment, but RO brine discharge is a big issue. Membrane distillation (MD) has been proposed to solve this problem by significantly increasing the water recovery ratio, and recovering minerals. However, membranes with high hydrophobicity targeting for MD, particularly for vacuum membrane distillation (VMD) are still scarce. Hyflon AD is a novel candidate for fabricating membranes for MD. In this paper, the effects of membrane fabrication parameters, such as coating time, heat treatment and pre-filling were investigated and optimized. Membrane morphology, mechanical properties and VMD performance of the composite membranes were tested. The results showed that the hydrophobicity and elongation at break of the membrane were significantly improved after coating. The coating polymer concentration, coating time, heat treatment temperature and heat treatment time for the membrane coated by Hyflon AD40L and Hyflon AD40H, respectively were optimized. Monovalent alcohols can be excellent pre-filling agents to improve membrane performance. Separation performance of the membrane coated by Hyflon AD40H was better than that of the one coated by Hyflon AD40L.

Cui, X. Li, Y. Zhang, Z. Wang, A. Gugliuzza, F. Militano, E. Drioli, F. Macedonio, Testing of three different PVDF membranes in membrane assisted-crystallization process: influence of membrane structural-properties on process performance, Desalination, Volume 440, 15

August 2018, Pages 68-77.

Abstract

Throughout the world an intensified use of desalination for reducing current and future water scarcity is observed. Despite the enormous benefits of desalination processes, improvements are still required in terms of lower desalted water cost, higher productivity, better water quality and enhanced eco-sustainability of the desalination process. Environmentally sensitive concentrate management is today recognized as a significant hurdle to extensive implementation of desalination technologies. Membrane assisted crystallization (MCr) offers a suitable solution for redesigning desalination process through the treatment of brine streams for the production of salts and water. In this work, three different Hyflon/polyvinylidene fluoride (PVDF) composite membranes were tested in MCr operations. The coating of PVDF membranes with Hyflon allowed increasing membrane surface hydrophobicity. The latter is the membrane essential characteristic when MCr is implemented according direct contact membrane distillation configuration like in the present work. The aim was to analyze the MCr performance in terms of membrane chemical–physical properties and process operating conditions.

Ali, A., Quist-Jensen, C.A., Drioli, E., Macedonio, F., Evaluation of integrated microfiltration and membrane distillation/crystallization processes for produced water treatment, Desalination 434, 2018, 161-168.

Abstract

Proper management and treatment of produced water has emerged as a big challenge for oil and gas industry. Increasingly stringent environmental regulations and economic constraints are compelling the use of more advanced treatment methods. Membrane operations are gaining significant interest for this application due to their broad range of separation capabilities, high efficiency and low operational cost. Commercially less-adopted membrane operations, such as membrane distillation (MD) and membrane crystallization (MCr) are gaining significant interest for produced water treatment due to their almost concentration-independent performance and less fouling potential. The current study analyzes the performance of an integrated microfiltration (MF) and direct contact membrane distillation (DCMD)/membrane crystallization (MCr) system for freshwater and minerals recovery from produced water. Based on the experimental data, thermodynamic/exergetic/quantitative analyses have been performed. Performance of the integrated processes has been compared with the conventional multi-stage flash (MSF) in terms of process intensification metrics.

Conidi, C., Drioli, E., Cassano, A., Membrane-based agro-food production processes for polyphenol separation, purification and concentration, Current Opinion in Food Science, 2018, vol 23, 149-164.

Abstract

Polyphenols, one of the main classes of secondary metabolites derived from plants, have received more and more attention in recent years due to their bioactive functions. Consequently, the interest in the extraction and separation of such compounds from agro-food sources has remarkably grown. Membrane processes can be considered leader technologies and very efficient unit operations in the recovery of food polyphenols. In this review, the main properties and fundamentals of pressure-driven membrane processes and membrane contactors are first presented. Then, specific applications for the separation, purification and concentration of polyphenols from agro-food products and by-products are analyzed and discussed, emphasizing the key technological advantages and improvements over conventional separation technologies.

C. Rizzuto, G. Pugliese, M.A.Bahattab, S.A.Aljlil, E. Drioli, E.Tocci, Multiwalled carbon nanotube membranes for water purification, Separation and purification technology, 2018, 193, 378-385.

Abstract

For the development of advanced membrane technologies, a good understanding of the materials properties and their transport mechanisms, as well as the realization of innovative functional materials with improved properties, are key issues. Due to their attractive permeability characteristics, various nano-structured RO membranes were proposed with the incorporation of carbon nanotubes. The growth in computational power has now made possible simulating tubes with characteristics closer to the real material, providing novel insights in the water flux to tube structure relationship. However, the understanding of the effect of the different number of walls, remains challenging and as a result, a deeper understanding is needed of how these changes can affect the performance of the membrane at the molecular level. To address this issue, molecular dynamic simulation (MD) is well known to be a powerful tool to enhance the understanding of nanoscale systems. This theoretical work provides new insights on the effect of walls in Multi Walled Carbon nanotube membranes, as model case of a CNT nanocomposite RO membrane, for desalination applications. Specifically, two types of vertically aligned multi Walled Carbon Nanotube membranes, MWCNT (6,6) and MWCNT (8,8), were analyzed theoretically by means of non-equilibrium Molecular Dynamics simulations, in order to study the influence of the number of walls on permeation of reverse osmosis simulations. A comparison of the two membranes formed by using differently sized tubes give us the estimation of the level of desalination and efficiency. The carbon nanotube membranes were modeled using two graphene sheets and single walled (SW), double walled (DW), three walled (TW) for both (6,6) and (8,8) configurations, and six walled (6W) for (6,6). Simulations were conducted with a hydrostatic pressure difference to investigate the ion rejection and water conductance in each membrane system. MWCNT (6,6) are very selective to ions whilst MWCNT (8.8) were more permeable to water. The different behaviour was justified in terms of the different size of entrance of CNT with a cooperative effect due to numbers of walls of CNT and the hydrophobic effect of the graphene layers. A good agreement is found if we compare our system with some functionalized SWCNT (8,8) (Corry, 2011) and with that of protein aquaporin-1 (Zhu et al., 2004). As the number of walls is augmented, the water conductance followed the same trend with a general performance greater than commercial reverse osmosis membranes (Corry, 2011). Under the conditions of our simulations, it appears that the MWCNT (8,8), particularly with DW (8,8) and TW(8,8) could offer an improvement over current generation membranes in terms of water conductance with a relatively good compromise between water conductance and salt rejection.

Y. Fan, E. Drioli, K. Fu, M. Qiu, X. Chen, X. Feng, Tubular hydrophobic ceramic membrane with asymmetric structure for water desalination via vacuum membrane distillation process, 2018, Desalination, Volume 443, Pages 212-220.

Abstract

A porous ceramic membrane without water wetting is essential for the application of water desalination in membrane distillation. In this study, we report a hydrophobic tubular asymmetric alumina membrane that was modified by grafting hexadecyltrimethoxysilane (C16) molecules. The grafting efficiency and hydrophobicity of the grafted membrane were characterized by its morphology, contact angle and FTIR spectrum, as well as the changes in terms of nitrogen permeance and pure water flux over various pressures. Four kinds of tubular asymmetric alumina membranes were employed in the vacuum membrane distillation (VMD) process. The effects of membrane thickness and pore size on the water flux or salt retention were investigated. The mass transport resistance in substrate was non-negligible and sometimes could be the main contributor to the total mass transport resistance. The membrane with a top layer thickness of 20 μm, pore size of 150 nm and support pore size of 3.2 μm was appropriate in the VMD process. After >1000 min desalination, the permeate flux and salt rejection were maintained as high as at the beginning, i.e., approximately 30 kg·m−2·h−1 and 99.9%, respectively.

Recent Advances in Atomic Layer Deposition (ALD)

by Markku Leskelä, Member EUAS

Short Biography

Department of Chemistry, PO Box 55, University of Helsinki, FI-00014 Helsinki, Finland

Markku Leskelä (www.helsinki.fi/kemia/epaorgaaninen/personnel/leskela.htm) completed the PhD in 1980 in Helsinki University of Technology. After working in University of Oulu and University of Turku as associate and full professor, he was nominated as professor of inorganic chemistry at University of Helsinki in 1990. His research activities include thin films and other nanostructured materials made by various chemical methods (Atomic Layer Deposition, electrodeposition and Successive Ionic Layer Adsorption and Reaction) for various applications in micro- and optoelectronics. The studies include all stages in film growth from precursor synthesis to applications. His other research topic is catalysis where the focus is in activation of small molecules by metal complexes in homogeneous systems. He has co-authored 700 original peer reviewed papers, 60 reviews and holds more than 30 patents. His h-index is 71 (ISI Web of Science). In 2004 he was nominated as ISI Highly Cited Author in the field of materials science. He has had several positions of trust in the University of Helsinki from which member of the board of trustees (2010-2017) is the most important. He is an active member in many Finnish and foreign professional societies. He is a member of three Finnish scientific academies and a board member of several foundations.

Principle of Atomic Layer Deposition (ALD)

ALD is a modification of chemical vapor deposition (CVD) with the difference that film growth takes place in a cyclic manner. Normally one growth cycle consists of four steps: 1) Exposure of the first precursor (often metal containing precursor), 2) purge of the reaction chamber, 3) exposure of the second precursor (non-metal precursor), and 4) a further purge of the reaction chamber (Figure 1) [1]. In each cycle equal amount of material is deposited on the surface. The growth cycles are repeated as many times as required for the desired film thickness. Depending on the process and the reactor design, one cycle can take time from 0.5 s to a few seconds, and may deposit between 0.1 and 3 Å of film material. The cycle time depends particularly on the aggressiveness of the film-formation reaction (negative ΔG value). The film thickness obtained per cycle may depend on the size of the precursor molecule (steric hindrance) and the number of adsorption sites at the surface.

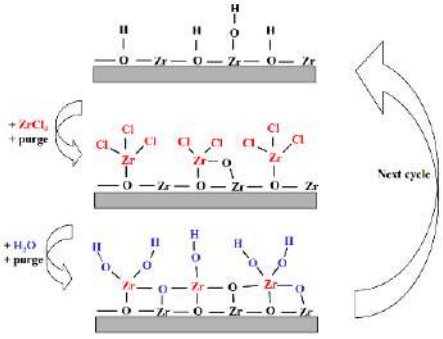

Fig. 1 An ALD deposition cycle showing schematically the deposition of ZrO_2 films from $ZrCl_4$ and H_2O.

In a good ALD process each exposure and purge step is complete, i.e. the precursor molecules chemisorb or react with the surface groups saturatively. Under these saturative reaction conditions the film growth is self-limiting meaning that the amount of film material deposited in each reaction cycle is constant. The self-limiting growth mechanism brings several advantages to ALD: 1) Film thickness depends only on the number of reaction cycles, which makes the thickness control

accurate and simple; 2) unlike CVD, there is less need of reactant flux homogeneity, which gives large area (large batch and easy scale-up) capability, excellent conformality i.e. the film follows exactly the morphology of the substrate (Figure 2) and reproducibility. The use of highly reactive precursors results in pure films being deposited at relatively low temperatures. The ALD processing window is often wide, which makes the process insensitive to small changes in temperature and precursor flows, and allows the processing of different materials to multilayer structures in a continuous process (Figure 3).[3]

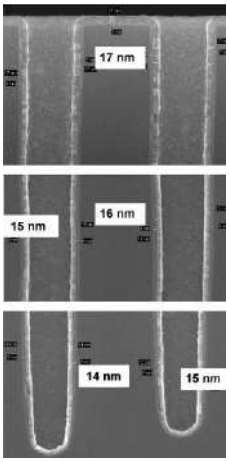

Fig. 2 Cross-sectional SEM images of a ZrO_2 film grown by the $CpZr(NMe_2)_3/O_3$ process into 60 : 1 aspect ratio trenches. The upper image shows the top part of the trench, those below the middle and bottom parts. The trench opening is 115 nm and depth 6.75 mm. Labels denote the ZrO_2 film thicknesses. [2]

ALD processes have been reported for a few hundred materials and number of processes is approaching 1500 [4]. The most common materials deposited by ALD are oxides but numerous processes exist for nitrides, chalcogenides and elements. The variety of metal precursors is wide ranging from elements and simple metal halides to complicated heteroleptic organometallic compounds. The selection of non-metal precursors is more limited, the simple hydrides being the most common molecules used. Thermal ALD is relying on thermal energy as driving force for surface reaction. For many compounds (nitrides, carbides, borides) and elements it is impossible to find precursor combination that produces the desired material at reasonable temperatures (< 500 ^oC). Different plasma - enhanced systems have been developed for those materials. [5] PE-ALD processes allow the deposition of thin films at low temperatures.

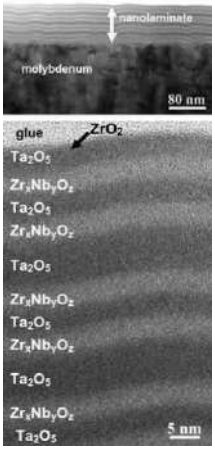

Fig. 3 Transmission electron microscope images of Ta_2O_5– $Nb_xZr_yO_z$ nanolaminates as-deposited at 275 °C. [3]

Applications of ALD

ALD technology was developed for manufacturing AC driven thin film electroluminescent (EL)

displays [6]. Monochromic yellow-black displays based on ZnS:Mn luminescent layer sandwiched between dielectrics and electrodes has been manufactured industrially by ALD continuously since 1984. Besides the luminescent layer, the high-quality oxide layers made by ALD have had an important role as dielectrics and passivation layers in the success of the AC driven thin film EL displays.

Microelectronics has been the major driver for ALD technology for the past twenty years. This development started in the late 1990's when it became obvious that the continuation of Moore's law will depend on an introduction of new materials and their deposition methods to the IC technology. ALD could respond to the requirements for the deposition of atomic level accuracy in thickness control, uniformity over the increasing wafer sizes and conformality over the increasingly complex device structures.

High-k dielectric materials as both alternative gate oxides in metal-oxide-semiconductor field effect transistors (MOSFET) and capacitor dielectrics in dynamic random access memories (DRAM) have been in the central role in microelectronics applications of ALD. DRAMs require increasingly more complex three-dimensional capacitor structures to ensure the required storage cell capacitance despite the ever decreasing memory cell areas. The aspect ratios are so high that ALD is needed for the high-k oxide deposition and ALD has indeed become a mainstream for capacitor dielectric deposition. The dielectric material of choice is today a ZrO_2-Al_2O_3-ZrO_2 nanolaminate [7].

Intel reported 2007 that they made a historic change of materials into the high-k dielectric – metal gate electrode stacks in MOSFETs. The gate dielectric was reported to be ALD made hafnium oxide based material. Since that the ALD high-k became in use in most of the MOSFETs and change from planar transistor structure to three-dimensional structures like FinFETs makes the use of ALD in processing unavoidable. [7]

The third use of ALD in microelectronics is focused on metal films. They could be used in interconnects, seed layers for copper or tungsten CVD deposition, and gate metal electrodes. In non-volatile memories – flash and phase change memories – ALD is potential method and the shrinking of device sizes and evolving of structures to three-dimensional favor ALD. At the moment microprocessor fabrication involves 20-30 ALD steps.

Being highly conformal and uniform, the ALD coatings can provide efficient sealing of substrates with basically any shape. ALD Al_2O_3 films were used in protective purposes already in the EL displays and is now used in many applications for example in jewelry production. With thicknesses as low as about 10 nm the ALD Al_2O_3 films have been found effective in preventing silver tarnishing. A robust process, inexpensive precursors (trimethyl aluminum plus water), and batch processing with 2000 pieces ensure the cost effectiveness of the process. There are many other applications too where ALD is used in industrial scale in passivation and encapsulation. Silicon based solar cells is a good example of the former [8] and OLED displays from the latter application area [9]. Conformality of films is the motivation for the use of ALD is MEMS preparation and the films may have different functions, such as wear resistant, lubricating, anti-stiction, insulating, or charge dissipating. [7]

Recent trends in ALD research and applications

ALD allows high precision coating of substrates with different size and shape including deep trenches and narrow pores. Therefore ALD can be used for coating of different nano-objects, such as nanopores, nanotubes, nanowires, nanoparticles and nanostructured surfaces. [3,10]. First other techniques are needed for preparation of the nanotemplate and then ALD is used to modify the nanosurfaces, either passivating the surface or bringing new functionalities. Intensity of nanomaterials research is increasing which also gives boost for ALD process research [11]

One very strongly evolving area in ALD research is that focused on energy technology materials. They involve materials for energy conversion (solar cells), energy storage (Li ion batteries, supercapacitors) and usage of energy (fuel cells). [12] There are also other energy applications for example photoelectrochemical water splitting and photocatalysis where suitability

of ALD deposited materials has been studied. [13,14] In silicon solar cells thin ALD Al_2O_3 films are used for passivation as mentioned above. [8] In thin film solar cells ALD could be used in all roles: absorbers, transparent conductors and buffer layers. Best results have been obtained for devices where light absorbing layers have been prepared by other techniques and ALD for buffer layers (In_2S_3, Zn(O,S), $Zn_{1-x}Sn_xO_y$). [15,16] In lithium ion batteries ALD has been utilized in protection of electrodes. A huge improvement can be seen in lifetime of the electrodes coated with few nanometer ALD oxide film. [17]. In microscale batteries ALD could be beneficial also in preparation of solid electrolyte. [18] From the different fuel cell types solid oxide fuel cells (SOFC) and especially those working at intermediate temperatures have mostly been focused in the ALD research. Again there are different places were ALD could be applied: electrodes, electrolyte, interface layers, barrier or protecting layers, and catalyst. [19]

Molecular Layer Deposition (MLD) is a variant from traditional ALD. MLD combines inorganic and organic precursors resulting in hybrid thin films (Figure 4). Combining inorganic and organic molecules gives endless possibilities to vary the structure and properties of the materials. The MLD materials have interesting elastic and optic properties that may find important applications.

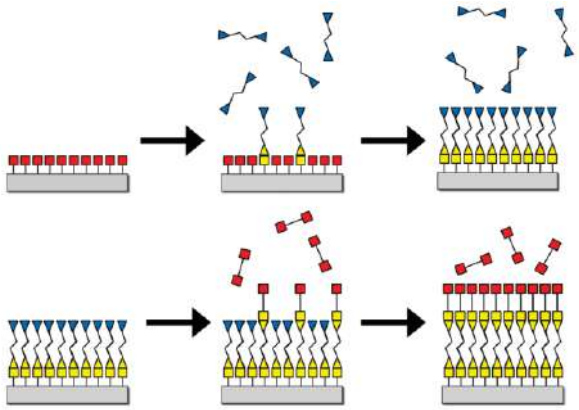

Fig. 4 Schematic of the MLD method based on sequential, self-limiting surface reactions of inorganic and organic molecules. [20]

Yet, a new active research area of ALD can be mentioned, namely two-dimensional transition metal dichalcogenides (TMDC). Thin films or monolayers of TMDC 2D materials have received enormous amount of attention due to their unique properties which are not seen in their bulk form. This is due to quantum confinement effects and the weakness of interlayer interactions in TMDCs. Bandgaps of these materials can be tuned by many ways such as thickness, strain, and functionalization. Molybdenum disulfide (MoS_2) is the most extensively studied TMDC material and it has been studied as a channel material in field-effect transistors as well as phototransistors and other optoelectronic devices. MoS_2 has also shown promise in catalysis, batteries, photovoltaics, and sensors. The bottle-neck in the large use of 2D TMDCs is the lack of scalable, low-temperature process for high-quality, large-area 2D materials (films). Atomic Layer Deposition (ALD) could be a solution for these problems. ALD processes have already been developed for several TMDCs and their properties characterized as seen in the recent review [21]. ALD of 2D material is still very immature and strong development can be expected.

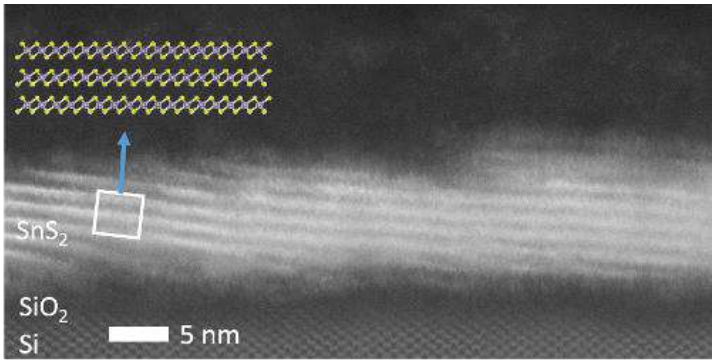

Fig. 5 Cross-sectional transmission electron microscopy image of a 6 nm thick SnS_2 film. [22]

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Innovative Contributions in Inorganic Materials Chemistry

by Glen Deacon, Member EUAS

Short Biography

Glen Deacon graduated BSc(Hons) (HI) and PhD from the University of Adelaide (CSIRO and AAEC Scholarships, an ICIANZ Fellowship, and the Senior Tutorship at Lincoln College). Postdoctoral research work was carried out with Professor Sir Ronald Nyholm FRS at University College London (CSIRO Overseas Scholarship, ICI Fellowship) with additional collaboration with Professor Alwyn Davies FRS (UCL) and Dr John Green (NPL Teddington).

He was appointed to a lectureship at Monash in 1966, and received accelerated promotion to Senior Lecturer (1971) and Reader (1975). For his research work on Main Group Element Chemistry he was awarded the DSc degree of the University of Adelaide in 1972. He became a Fellow of the Royal Australian Chemical Institute in 1975. In 1994 he was appointed to a Personal Chair in Chemistry and was Professor of Chemistry from 2002-2012 when he was appointed Professor Emeritus. In 2005-6, he was also a Senior Adviser in the Monash Research Office.

Glen Deacon has achieved international recognition in several areas of Inorganic and Inorganic Materials Chemistry, particularly the Chemistry of Main Group Elements, Rare Earths, Precious Metals (including platinum anti-cancer compounds), Small Cyano Anions, New Materials (semi-conductor dopants and precursors) and Corrosion Inhibitors. He has received extensive research funding both alone and in research teams, e.g. from ARC (more than 50 grants including support from the Centre for Green Chemistry), ACCV, and GIRD, and is involved in extensive National and International (e.g. Germany, UK, France, Japan) research collaboration. He has supervised or jointly supervised 24 postdoctoral workers, 16 research assistants, and 50 PhD, 4 MSc, 6 MEnvSci and over 70 BSc(Hons) graduates. Over 550 papers have been published in refereed journals and several book chapters have been published. He has over 20000 citations averaging 32/ article and an h index of 53. Considerable consulting/contract research has been carried out for industry and government agencies, and a patent is in commercial use.

*Glen Deacon held a Visiting Lectureship at the University of Western Australia (1991), Guest positions at Universität Dortmund, Technische and Frei Universität Berlin, Universität Hannover, Universität Leipzig, Universität Tübingen, Universität Stuttgart, Universität Duisburg, KIT and Universität zu Köln, and was a Senior Academic Visitor, Queen Mary College, University of London and James Cook University, and has been Visiting Professor and Foundation Lecturer in Inorganic Chemistry, University of Sydney. Since 1987, he has given over 200 invited lectures/seminars at National and International (UK, USA, Germany, Netherlands, Eire) Conferences, Universities, Research Organisations etc. In 2006, he was awarded the Terrae Rarae Prize for Rare Earth Chemistry and in 2007 received the Burrows Award of the Royal Australian Chemical Institute for Inorganic Chemistry. From 2002-2004, he served on the Committee of Experts of the Australian Research Council. In 2012, the SO_3 elimination synthesis of organometallic compounds discovered by the Deacon group in the 1970s, was named the Deacon reaction (Organometallics, 2012, **31**, 1801).*

Reactivity of bulky formamidinatosamarium(II or III) complexes with C=O and C=S bonds

Glen B. Deacon, Peter C. Junk, Jun Wang and Daniel Werner

Inorg. Chem., 2014, 53, 12553-12563

Abstract

The preparation of a new heterobimetallic samarium(II) formamidinate complex and selected reactions of samarium(II) and one samarium(III) formamidinate complexes with benzophenone or CS_2 are discussed. Treatment of the tris(formamidinato)samarium(III) complex [Sm(DippForm)$_3$] **1** (DippForm = *N,N′*-bis(2,6-diisopropylphenyl)formamidinate, (CH(N(C$_6$H$_3$-^{i}Pr-2,6)$_2$) with potassium graphite in toluene, yielded the dark brown heterobimetallic formamidinatosamarium(II)/potassium complex [KSm(DippForm)$_3$]$_n$ **2**. Divalent **2**, a Lewis base solvent free homoleptic species, differs significantly from the related heteroleptic formamidinatosamarium(II) complex [Sm(DippForm)$_2$(thf)$_2$] **3** with respect to its constitution, structure and reactivity towards benzophenone. Whilst **2** reacts giving complex **1**, the reaction of **3** with benzophenone generates highly unusual [Sm(DippForm)$_2$(thf){μ-OC(Ph)=(C$_6$H$_5$)C(Ph)$_2$O}Sm(DippForm)$_2$] (C$_6$H$_5$ = 1,4-cyclohexdiene-2,5-enyl) **4**. The formation of **4** highlights a rare C-C coupling between a carbonyl carbon and the carbon at the *para*-position of a phenyl group of the OCPh$_2$ fragment. An analogous reaction of [Yb(DippForm)$_2$(thf)$_2$] gives an isostructural complex **4Yb**. **3** reacts with carbon disulfide forming a light green dinuclear formamidinatosamarium(III) complex [{Sm(DippForm)$_2$(thf)}$_2$(μ-η^2(C,S):κ(S′,S″)-SCSCS$_2$)]$_2$ **5** through an unusual C-S coupling by an amidinatolanthanoid species giving the thioformylcarbonotrithioate ligand. The trivalent organometallic [Sm(DippForm)$_2$(CCPh)(thf)] complex activates the C=O bond of benzophenone by an insertion reaction, forming light yellow [Sm(DippForm)$_2$\{OC(Ph)$_2$C$_2$Ph\}(thf)] **6** as a major product and light yellow unsolvated [Sm(DippForm)$_2$\{OC(Ph)$_2$C$_2$Ph\}] **7** as a minor product. Molecular structures of complexes (**2**, **4**-**7**) show that □(*N,N′*) bonding between a DippForm and samarium atom exists in all compounds, but in **2**, DippForm also bridges K and Sm by 1κ(N):2κ(N′) bonding and two 2,6-di-*iso*propylphenyl groups are η^6--bonded to potassium.

Bulky Ytterbium Formamidinates Stabilise Complexes With Radical Ligands

Daniel Werner, Xuefei Zhao, Stephen P. Best,[] Laurent Maron, [] Peter C. Junk, and Glen B. Deacon

Chem.Eur.J. 2017, 23, 2084-2102

Abstract

Divalent [Yb(DippForm)$_2$(thf)$_n$] (n = 2 (**1a**), or 1 (**1b**); DippForm = *N,N′*-bis(2,6-diisopropylphenyl)formamidinate) complexes were treated with the ketones: 9-fluorenone (FN), or 2,3,4,5-tetraphenylcyclopentadienone (TPC, tetracyclone), giving *ketyl*† complexes: [Yb(DippForm)$_2$(fn˙-*O*)(thf)] (**2**), and [Yb(DippForm)$_2$(tpc˙-*O*)] (**4**) respectively. Both complexes were characterised by X-ray crystallography, and were stable in both polar and non-polar solvents, an uncommon trait for rare-earth *ketyl* complexes. When perfluorobenzophenone (PFB) was treated with either **1a** or **1b**, the formed *ketyl* species was only transient, and was followed by rapid decomposition via a C–F activation pathway, leading to the isolation of [YbF(DippForm)$_2$(thf)] and a highly unusual fluoride/oxide bridged species: [Yb$_5$F$_6$O$_2$(DippForm)$_5$]. To investigate the reactivity of the tpc˙-*O ketyl* complex, **4** was treated with oxidants (CS_2, Se), reducing agents (Mg^0, [SmI$_2$(thf)$_2$]), and KH. Thus **4** was oxidised to TPC by Se, or further reduced to a di-anion (1-oxido-2,3,4,5-tetraphenyl-cyclopentadianide(2-), ({C$_5$Ph$_4$}–*O*)$^{2-}$ by [SmI$_2$(thf)$_2$], giving dimeric [{SmI({C$_5$Ph$_4$}-*O*)(thf)$_2$}$_2$] and monomeric complexes [YbI(DippForm)$_2$(thf)] and [YbI$_2$(DippForm)(thf)$_2$]. Treatment of **4** with KH led to a ligand exchange process giving an unusual di-*ketyl* species [Yb(DippForm)(tpc˙-*O*)$_2$(thf)$_2$], which contained two *cisoid* tpc˙-*O*$^-$ ligands in very close proximity. The reduction of 1,2-diketones was also examined. Complex **1a** (or **1b**) was treated with one equivalent of either 3,5-di-*tert*-butyl-benzo-1,2-quinone (TBBQ), phenanthrene-9,10-dione (PHEN), or acenaphthalene-1,2-dione (ACEN), giving *ketyl* complexes: [Yb(DippForm)$_2$(tbbq˙-*O*$_2$)], [Yb(DippForm)$_2$(phen˙-*O*$_2$)], and [Yb(DippForm)$_2$(acen˙-*O*$_2$)(thf)] (**9**).

An unsolvated derivative of **9**, namely [Yb(DippForm)$_2$(acen˙-O_2)] (**10**) was obtained when **9** was crystallised from PhMe. The *ketyl* character of relevant ligands was supported by X-ray crystallography (e.g. the elongation of the C–O bond lengths for those derived from ketones, and resonances stabilisation over the OCCO bite for those from diketones), and (with the exception of **4**) through ESR spectroscopy.
[†]*Ketyl:* A radical anion containing a C˙-O$^{(-)}$ group. *Abbreviations: FN: 9-fluorenone; fn˙-*O*˙:9-Fluorenone *ketyl*; PFB: perfluorobenzophenone; TPC: 2,3,4,5-tetraphenylcyclopentadienone, tpc˙-*O*˙: 2,3,4,5-tetraphenylcyclopentadienone *ketyl*; ({C_5Ph_4}-*O*)$^{2-}$: 1-oxido-2,3,4,5-tetraphenyl-cyclopentadienide(2$^-$). TBBQ: 3,5-di-*tert*-butyl-benzo-1,2-quinone; tbbq˙-O_2˙$^-$: 3,5-di-*tert*-butyl-benzo-1,2-quinone *ketyl*; PHEN: phenanthrene-9,10-dione, phen˙-O_2˙$^-$: phenanthrene-9,10-dione *ketyl*; ACEN: acenaphthalene-1,2-dione; acen˙-O_2˙$^-$*:* acenaphthalene-1,2-dione *ketyl.*

Can bismuth replace mercury in redox transmetallation/protolysis syntheses from free lanthanoid metals?

Zhifang Guo, Victoria Blair, Glen B. Deacon, and Peter C. Junk

Chem. Eur J 2018, 24, 17464-17474

Abstract

Tris(pentafluorophenyl)bismuth has been examined as a potential replacement for diarylmercurials in redox transmetallation/protolysis (RTP) syntheses of reactive rare earth compounds from free rare earth metals, $HgAr_2$, and a proligand HL. Thus, the lanthanoid pyrazolates, [Ln(Ph_2pz)$_3$(thf)$_3$] (Ph_2pz = 3,5-diphenylpyrazolate; Ln = La, **1**, Ce**, 2**, Nd, **3**, Tb, **4**; thf = tetrahydrofuran), [Ln$_2$(Ph_2pz)$_4$(OMe)$_2$(dme)$_2$]·2dme (Ln = Ho, **5**, Er, **6**, Tm**, 7**, Lu, **8**; dme = 1,2-dimethoxyethane), [Ln(Ph_2pz)$_3$(dme)$_2$] (Ln = Dy, **9**, Sm, **10**), [Ln(*t*Bu_2pz)$_3$(thf)$_2$] (*t*Bu_2pz = 3,5-di-*tert*-butylpyrazolate; Ln = La, **11**, Ce, **12**, Sm, **13**, Gd, **14**, Dy, **15**, Ho, **16**, Tm, **17**, Yb, **18**, Lu, **19**), [Ln(ttfpz)$_3$(thf)$_3$] (ttfpz = 3-(2´-thienyl)-5-(trifluoromethyl)pyrazolate; Ln = La, **20**, Sm**, 21**), and [Er(PhMepz)$_3$(thf)$_2$] **22** (PhMepz = 3-phenyl-5-methyl-pyrazolate) have been prepared in good yields by redox transmetallation/protolysis reactions employing lanthanoid metals, trispentafluorophenylbismuth [Bi(C_6F_5)$_3$]·0.5diox (diox = 1, 4-dioxane) in donor solvents. This is a new and efficient synthetic route in which Bi(C_6F_5)$_3$ replaces the commonly used Hg(C_6F_5)$_2$ or $HgPh_2$ and provides proof of concept for the method. [Ln$_2$(Ph_2pz)$_4$(OMe)$_2$(dme)$_2$]·2dme (**5-8**) complexes are derived from C–O bond activation of dme on crystallization of the initial products from this solvent and are dimeric methoxide-bridged species. Other structures are monomeric with η^2-bound pyrazolate ligands and nine-coordinate metal atoms for complexes **1-4**, **9-10** and **20-21**, and eight-coordinate metal atoms *for complexes **11-19** and **22**.*

Divalent tetra- and pentaphenylcyclopentadienyl europium and samarium sandwich and half-sandwich complexes: synthesis, characterization and remarkable luminescence properties

Toby D. M. Bell, Rosalind P. Cox, Daisy P. Daniels, Glen B. Deacon, Florian Jaroschik, Peter C. Junk Rory P. Kelly, Xavier F. Le Goff, Gilles Lemercier, Agathe Martinez, Jun Wang and Daniel Werner

Organometallics 2015, 34, 5524-5536

Abstract

Redox-transmetalation/protolysis (RTP) reactions between an excess samarium or europium metal, $HgPh_2$ and two equivalents of C_5Ph_5H afforded the symmetrical decaphenylmetallocenes, $[Ln(C_5Ph_5)_2]$ (Ln = Sm, Eu). Analogous reactions with $C_5Ph_4H_2$ gave the octaphenylmetallocenes, $[Ln(C_5Ph_4H)_2(solv)]$ (Ln = Sm, solv = thf; Ln = Eu, solv = dme)]. Recrystallization of the known complex, $[Yb(C_5Ph_4H)_2(thf)]$, from dme yielded the solvent-separated ion pair, $[Yb(dme)_4][C_5Ph_4H]_2$. A rare heteroleptic samarium bromide complex, $[Sm(C_5Ph_5)(\mu\text{-}Br)(thf)_2]_2$, was synthesized from the RTP reaction between an excess of samarium metal, PhHgBr and C_5Ph_5H, while $[Sm(C_5Ph_4H)I(thf)_3]$ was prepared from the reaction between equimolar amounts of $[Sm(C_5Ph_4H)_2(thf)]$ and $SmI_2(thf)_2$. $[Eu(C_5Ph_5)_2]$ and $[Eu(C_5Ph_4H)_2(dme)]$ exhibit remarkable luminescence properties with quantum yields of 45 % and 41 % respectively. In addition, both complexes display very long lifetimes.

Enhancing the Value of Free Metals in the Synthesis of Lanthanoid Formamidinates. Is a Co-Oxidant Needed?

Glen B. Deacon , Peter C. Junk, and Daniel Werner

Chem. Eur . J. 2016, 22, 160-173

Abstract

Treatment of *N*,*N*′-bis(aryl)formamidines (ArFormH), *N*,*N*′-bis(2,6-difluorophenyl)formamidine (DFFormH) or *N*,*N*′-bis(2,6-diisopropylphenyl)formamidine (DippFormH), with europium metal in CH_3CN is an efficient synthesis of the divalent complexes: $[\{Eu(DFForm)_2(CH_3CN)_2\}tilted_2]$ (**Eu1**) or $[Eu(DippForm)_2(CH_3CN)_4]$ (**Eu2**). The synthetic method was extended to ytterbium, but the metal required activation by addition of Hg^0. With DFFormH in CH_3CN, $[\{Yb(DFForm)_2(CH_3CN)\}_2]$ (**Yb1**) was obtained in good yield, and $[Yb(DFForm)_2(thf)_3]$ (**Yb3**) was obtained from a synthesis in CH_3CN/thf. Thus, this synthetic method completely circumvents the use of either salt metathesis, or redox transmetallation / protolysis (RTP) protocols to prepare divalent rare-earth formamidinates. Heating **Yb1** in PhMe (C_6D_6) resulted in decomposition to trivalent products, including one from a CH_3CN activation process. For a synthetic comparison, divalent ytterbium DFForm and DippForm complexes were synthesised by RTP reactions between Yb^0, $Hg(R)_2$ (R = Ph, C_6F_5), and ArFormH in thf, leading to the isolation of either $[Yb(DFForm)_2(thf)_3]$ (**Yb3**), or the first five coordinate rare-earth formamidinate complex $[Yb(DippForm)_2(thf)]$ (**Yb4b**), and, from adjustment of the stoichiometry, *trivalent* $[Yb(DFForm)_3(thf)]$ (**Yb6**). Oxidation of **Yb3** with benzophenone (bp), or halogenating agents ($TiCl_4(thf)_2$, Ph_3CCl, C_2Cl_6) gave $[Yb(DFForm)_3(bp)]$ or $[Yb(DFForm)_2Cl(thf)_2]$ respectively. Furthermore, the structural chemistry of divalent ArForm complexes has been substantially broadened. Not only have the highest and lowest coordination numbers for divalent rare-earth ArForm complexes have been achieved in **Eu2** and **Yb4b** respectively, but also dimeric **Eu1** and **Yb1** have highly unusual ArForm bridging coordination modes, either perpendicular μ-1κ(*N*:*N*′):2κ(*N*:*N*′) in **Eu1**, or the twisted μ-1κ(*N*:*N*′):2κ(*N*′:*F*′) DFForm coordination in **Yb1**, both unprecedented in divalent rare-earth ArForm chemistry and in the wider divalent rare-earth amidinate field.

Major Contributions in Materials Science Engineering

by Folker H. Wittmann, Member EUAS

Short Biography

Born April 20th 1936 in Karlsruhe, Germany, I visited the Markgrafen Gymnasium (high school) in Karlsruhe Durlach. Then I studied Physics first at Karlsruhe University of Technology (today KIT). After the Vordiplom (Bachelor) I changed to Munich University to continue my studies in Physics until Diplom (Master degree). In 1961 I started with PhD studies at Munich University of Technology under supervision of Professor Maier-Leibnitz. The topic of my thesis was "Angular Distribution of Resonant Scattered Gamma-rays" (Mößbauer Effekt). As an assistant professor I continued at Munich University of Technology to study Materials Science in 1965. I finished my habilitation in 1969. In 1976 I received the RILEM Medal for my fundamental research on cement-based materials. From 1976 to 1980 I was full professor at Delft University of Technology, The Netherlands, and from 1980 to 1989 I had the same position at Swiss Federal Institute of Technology in Lausanne (EPFL, Ecole Polytéchnique Fédérale de Lausanne). In 1985 I was nominated Advisory Professor of Tongji University, Shanghai, China. Finally, I was professor for Building Materials Science and director of the Laboratory for Building Materials Science of Swiss Federal Institute of Technology in Zurich (ETHZ) from 1989 to 2001. In 1998 I received an honorary doctorate (Dr. h. c.) from University of Essen. In 1990 I was elected as a Foreign Member of the Russian Academy of Technological Sciences. Starting in 2002 I continued my carrier as Academy Professor at Qingdao Institute of Architecture and Engineering in Qingdao, today Qingdao University of technology (QUT), China. In 2010 I received the International Science and Technology Cooperation Award of the Peoples Republic of China. In 2018 I was appointed as Tenured Honorary Professor of China Building Materials Academy (CBMA).

I published more than 500 papers in leading international journals and edited more than 20 Proceedings of International Conferences. I chaired a number of International Committees. My hobby is playing piano alone or with friends.

Major Research Activities

For my Master Thesis in theoretical optics I studied contrast transmission functions with and without apodization filters at Munich University. The topic of my PhD thesis at Munich University of Technology (TUM) was angular distribution of scattered gamma radiation (Mössbauer Effekt). Then I applied the Mössbauer Effect to study hydration of iron containing clinker phases in cement.

A wide field of activities was later the scientific investigation of creep and shrinkage of cement-based materials. The influence of adsorbed and capillary condensed water on creep and shrinkage was of primary interest for many years. In this context the role of surface energy of nano-particles in cement gel was studied in great detail. It could be shown that rate-theory is an excellent basis to better understand time-dependent deformations of concrete under load.

Fracture mechanics of composite materials became a major field of research in the early seventieths. Crack propagation under increasing load and under high constant load was studied theoretically and the theoretical approach was validated by experimental test series. Crack growth under high compressive load was of primary interest. In this context crack propagation in composite materials was studied in great detail, both theoretically and experimentally.

A now widely applied wedge splitting test to determine fracture energy of concrete was developed. This test method served later as basis for an international technical committee (RILEM TC 50-FMC) to formulate a standard method to determine fracture energy and strain softening.

In order to understand the interaction of nano-particles with adsorbed water films in hydrated cement van der Waals interaction was studied both theoretically and experimentally. The influence of adsorbed water films was of particular interest in order to predict long term properties of concrete.

Activation energy and activation volume of creep of hardened cement paste was studied in great detail.

Fluorescence, afterglow and thermo-luminescence of X-rayed clinker components and different cements were studied in detail. Results of these tests helped us to better understand details of properties of cement-based materials.

The physical background of capillary shrinkage of fresh and hardened concrete was formulated the first time and early age crack formation in concrete could be described in detail. These studies also helped to overcome a practical problem, namely early crack formation in young concrete, which was a wide spread and serious early damage observed on young concrete slabs.

Extensive theoretical and experimental studies were carried out to understand the influence of rate of loading on strength of concrete. A stochastic approach served as a theoretical basis for these studies.

The influence of moisture content and of change of moisture content on total deformation of concrete was studied in great detail. Many aspects which were known phenomenological could be explained and predicted quantitatively on this basis. These studies helped to increase service life of reinforced concrete structures significantly.

A numerical tool was developed to predict the behavior of concrete under different climatic environment. This approach now called “numerical concrete” was very helpful to understand the behavior of concrete under complex loading conditions. Results obtained by extensive experimental studies could be understood and interpreted correctly for the first time.

As a minor sideline the elastic modulus of calcium hydroxide was determined for the first time.

The physical basis of shrinkage mechanisms was another interesting project. It helped us to understand the complex origin of shrinkage of porous materials and how to modify and reduce shrinkage of cement-based materials. The influence of size of specimens on strength was a wide field of theoretical and experimental studies.

For the first time neutron radiography was applied to study the time dependent moisture distribution in porous building materials. This method proved to be extremely powerful to study capillary absorption of water and time-dependent moisture distributions during drying of water saturated porous materials such as concrete. The influence of crack formation on drying and water uptake was of particular interest. Neutron radiography was also applied to visualize penetration into cracked reinforced concrete and to visualize the length of the damaged zone in front of a real crack and penetration of water or salt solutions into the interface between concrete and steel reinforcement.

Water repellent treatment of the surface of concrete elements can be an efficient protection to avoid penetration of aggressive ions dissolved in water, such as chloride. FT-IR spectroscopy proved to be an excellent tool to check the influence of protective water repellent treatment.

In parallel to running experimental studies numerical models to simulate properties of concrete were developed. First two-dimensional models served to simulate crack formation in a composite material such as concrete. Later this model was extended to a 3D model. Three-dimensional numerical concrete provides us with the possibility of quantitative prediction of shrinkage for instance, or of crack formation under load.

Disjoining pressure in cement-based materials and in two sphere models was determined and results help us to better understand shrinkage mechanisms. The influence of alkali content on creep and shrinkage can be expressed quantitatively based on these observations.

In cooperation with an international technical committee (RILEM TC 246-TDC) numerous test series were carried out to study durability and service life of concrete structures exposed to environmental actions as for instance chloride penetration into the pore space of concrete under the simultaneous action of an applied mechanical compressive or tensile stress.

In another RILEM Technical Committee (RILEM TC FTC) the influence of a combination of freeze-thaw cycles and chloride penetration into concrete on service life of reinforced concrete structures is being studied. The aim of all RILEM technical committees is to prepare guidelines for national and international standards.

An Attempt to Adopt the Workflow the Automative & Aircraft Industry for the Design of Drug Delivery Vehicles

by Hans Leuenberger, Member EUAS

Short Biography

EDUCATION

1971	*Doctor of Philosophy (Nuclear Physics)* *University of Basel, Basel, Switzerland*
1967	*Diploma in Experimental Physics* *University of Basel, Basel, Switzerland*
1962	*Matura Type B (Latin, English, Mathematics) Realgymnasium, Basel*

SABBATICAL AND OTHER EXPERIENCE

1980	*Section Head, Pharmaceutical Research and Development* *Sandoz España, Barcelona ad interim (Spain)*
1979	*University of Michigan, Ann Arbor (worked with Prof. W. I. Higuchi, Prof. N. F. Ho and Dr. E. W. Hiestand)*
1973	*University of Hamburg, Germany (worked with Prof. H. Sucker)*

EMPLOYMENT HISTORY AND PROFESSIONAL EXPERIENCE

2017 - . Present	*Adjunct Professor* *College of Pharmacy of the University of Florida, Department of Pharmaceutics, 6550 Sanger Road, Orlando Campus at Lake Nona Medical City FL 32827*
2007 - Present	*Professor Emeritus of Pharmaceutical Technology* *University of Basel, Basel, Switzerland* *(actively supervised thesis research of additional 20 doctoral students and provided training to visiting international scholars on sabbatical until year 2011)*
Nov. 2007 -	*Founding Director of the Center for Innovation in Computer-aided Pharmaceutics (CINCAP llc.) in association with Dr. Maxim Puchkov; (www.cincap.ch)*
Nov. 2006 -	*Founder and CEO of the Institute for Innovation in Industrial Pharmacy, Ifiip llc., (Consulting Company, see www.ifiip.ch).*
1982 - 2006	*Professor and Director* *Institute of Pharmaceutical Technology, University of Basel, Basel*
1995 - 2004	*Professor and Chair* *Department of Pharmaceutical Sciences* *Institute of Pharmaceutical Technology, University of Basel, Basel*
1994 - 95	*Dean, Faculty of Natural Sciences, University of Basel, Basel* *and Founder of the Faculty Committee of Department Heads*
1988-1993	*Member of the Export Group 12 (Pharmaceutical Technology) of the European Pharmaceutical Commission, Strasbourg, France*
1980 - 1982	*Adjunct Professor of Pharmaceutical Technology* *Department of Pharmaceutical Sciences* *Institute of Pharmaceutical Technology, University of Basel, Basel*
1973-1982	*Group Leader, Pharmaceutical Research & Development* *Sandoz Ltd., Basel, Switzerland*
1971-1973	*Section Head, Preformulation and Analytical Research & Development* *Sandoz Ltd., Basel*

PROFESSIONAL AFFILIATIONS AND RELATED ACTIVITIES

2017 - Present	*Member, American Association for the advancement of Science (AAAS)*
2017 - Present	*Member of the European Union Academy of Sciences (EUAS)*
2006 -2011	*President* *Swiss Society of Pharmaceutical Sciences (SGPhW)* *Founded Swiss Academy of Pharmaceutical Sciences (SAPhS) by changing by-laws of SGPhW whereby Scientific Council of SGPhW became official SAPhS.*
2001	*Member, Board of Directors of CAETS (International Council of Academies of Engineering and Technological Sciences)*
1999 - 2001	*Member, Scientific Council of CASS (Conseil des Académies Scientifiques Suisses)* *[today = Board of Directors of Swiss Academies of Arts and Sciences(https://en.wikipedia.org/wiki/Swiss_Academies_of_Arts_and_Sciences)]*
1993 - 2001	*Vice President, Swiss Academy of Engineering Science*

1993 - 1999	*Member of the Board of CASS (Conseil des Académies Scientifiques Suisses) as Vice President of SATW.*
1993 - 1997	*Member, Peer Review Committees ETH, Zurich (1993), University of Groningen, Netherlands (1997) and Utrecht University, Utrecht, Netherlands (1997)*
1992 - 1996	*President, Scientific Council of the Swiss Academy of Engineering Science and Founder of Swiss Academy of Engineering Sciences (SATW) Lateral Think Tank*
1987 - Present	*Member of the Swiss Academy of Engineering Sciences (SATW)*

PROFESSIONAL HONORS, AWARDS AND RECOGNITIONS (major ones only)

2011	*Fellow of the Swiss Academy of Pharmaceutical Sciences*
2008	*Doctor of Philosophy (Ph.D.) (Honoris causa) awarded by Mendeleyev University of Chemical Technology of Russia (MUCTR), Moscow, Russia*
2007	*Doctor of Philosophy (Ph.D.) in Pharmaceutics (Honoris causa) awarded by Mahidol University, Bangkok, Thailand*
2007	*Honorary Member, Society of Pharmacists of the Canton of Basel-City (BAV, Baselstädtischer Apothekerverband)*
2007	*Honorary President, Cátedra Iberoamericana-Suiza de Desarrollo de Medicamentos, CISDEM, University of Seville, Spain (CISDEM organizes every year a Forum on the advancements of Pharmaceutical Technology in conjunction mostly with a major congress in one of the currently 16 member states of South-Middle Americas, Spain, Portugal and Switzerland.)*
2006	*Recipient of "50ht Anniversary Award of the Society of Powder Technology of Japan (SPTJ)" for distinguished achievements and outstanding contributions to promote the international cooperation in powder technology*
2006	*Recipient of "European Pharmacopoeia – Council of Europe Medal" in recognition of achievements in Pharmaceutical Technology*
2005	*Honorary Director, Russian Swiss Science and Education Center for Pharmaceutical and Biological Technologies at the Mendeleyev University of Chemical Technology of Russia*
2005	*Recipient of Certificate of Agglomeration Award in Recognition of the Outstanding Contribution to the Development of Agglomeration Sciences awarded by International Symposium on Agglomeration, Bangkok, Thailand (March 16-18)*
2004	*Recipient of Certificate of Appreciation for Outstanding Service awarded by The International Council of Academics of Engineering and Technological Sciences Inc., Washington DC (www.caets.org)*
2001 - 2006	*Member of the Scientific Advisory Board of the Grand École des Mines, Albi, France (www.enstimac.fr).*
2001	*Recipient of Award of Particulate Preparations and Design of the Society of Powder Technology of Japan, Kyoto, Japan*
2001 - Present	*Honorary member of the Swiss Academy of Engineering Sciences (SATW)*
2000	*Recipient of IPS Medal from Industrial Pharmacy Section of FIP (Féderation International Pharmaceutique)*
1998 - Present	*Corresponding Member of the Royal Academy of Pharmacy of Spain.*
1998 - Present	*International Member of the Russian Academy of Engineering Sciences.*
1997	*Recipient of Jörg Bider Medal of the Swiss Society of Pharmacists (SAV)*
1994	*Recipient of Innovation Award for New Process Technologies of the Governments Basel-City and Basel-Country.*
1994 - Present	*Honorary Member of the Swiss Society of Industrial Pharmacists ([GSIA)*
1993	*Recipient of AAPS Research Achievement Award in Pharmaceutical Technologies by American Association of Pharmaceutical Scientists (AAPS)*
1993	*Member, Expert Group 12 between 1988-93: the "European Pharmacopoeia - Council of Europe Medal".*
1990	*Fellow, American Association of Pharmaceutical Scientists (AAPS)*
1989	*Recipient of University of Helsinki Medal*

An Attempt to Adopt the Workflow the Automative & Aircraft Industry for the Design of Drug Delivery Vehicles

Duangmanee Maneerojpakdee, Ampol Mitrevej, Nuttanan Sinchaipanid, Jay Nowak, Hans Leuenberger

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Abstract

A prerequisite to adopt the workflow of the aircraft industry for the design of drug vehicles such as tablets consists in the availability of a F-CAD (Formulation-Computer Aided Design) platform to be able to design and test *in silico* the drug carrier vehicle. Such a workflow corresponds to a very rigorous interpretation of a“ Right, First Time” concept starting at Clinical Phase I. Based on a Quality by Design (QbD) approach it is important to follow ICH Q8 (R2) recommendations to explore the formulation design space *in silico* or in reality by manufacturing laboratory batches. The successful implementation of the workflow needs a harmonization of equipment. For this reason, the PressterTM equipment was applied for the development of a 80 mg Nifedipine extended release tablet formulation, simulating mechanically a high speed rotary press. Following the guideline of ICH Q8 R(2), the mathematical model that describes the properties of the tablet formulation was applied. Thus, the mathematical model of the 3×3 design served as a virtual design tool. Applying the software STAVEX 5.2 this tool proved to be very versatile. However, it was not possible to substitute all features of F-CAD of CINCAP.

Conclusions

The guidelines of ICH Q8(R2), especially, the use of experimental design for the exploration of the formulation design space including the application of STAVEX 5.2 for the *in silico* description of the important responses of the formulations in the complete design space are extremely fruitful. The PressterTM equipment used for the harmonization of processes and equipment shows to be an excellent PAT device to test the sensitivity of tablet formulations to the tableting speed. As an optimal 80 mg Nifedipine formulation, the following procedure is suggested: Direct compaction of an oblong tablet consisting of the formulation CR4/7 with the coordinates (x1 = -1, x2 = +0.5), i.e. x1 = 100 : 220 = ratio PVP K-30/EC [mg] and x2 = 65 : 35 = ratio MCC Sanaq burst/ MCC PH 102 [mg] with 55 mg Nifedipine per oblong tablet. After applying an aqueous solution of PVP/Nifedipine complex with 25 mg Nifedipine each tablet contains 80 mg API and 25 mg is released immediately. As an alternative for adding classically 0.5% Magnesium stearate an external lubrication system can be used.

The study shows clearly that in an industrial environment there is no time for basic research during the development phases. Thus, an industrial pharmacist cannot enjoy to study and explain interesting phenomena, which occur during the development phases. The motivation of a formulation scientist consists in achieving a high quality of the dosage form in a short time. Thus, time to market plays an important role. This looks to be just a commercial point of view but has a high societal impact if the number of successful introduction of new APIs and therapies is increased. This is the reason, why FDA pushes forward the concept of“ Right, First Time”. Such a holistic approach avoids losing sight of the wood for trees. Thus, for the advancement of pharmaceutical science a close cooperation between industry and academia is a prerequisite. Indeed, it is the task of academia or of a spin-off start-up company to develop the virtual tools for a better understanding of the processes and formulations. F-CAD as a virtual tool is able to serve as a“ learning suite” and is able to predict the important properties of a solid dosage form after calibration. The classical approach according to the guidelines of ICH Q8 (R2) describing the formulation design space needs much more laboratory experiments and is by nature retrospective as the prediction is primarily based on an interpolation with the formulation design space.

Already a simple 3×3 design with only 9 lab batches gives a helpful insight in the formulation design space. In this context, it is important to take into account the set theory. Thus, special actions are needed as shown in this present study if the relevant responses do not overlap in design space regions being disjoint. In order to avoid redundant experiments creating unnecessary costs the set theory urges that an originator company should start the first clinical trials with the same dosage form as marketed later.

Curiosity was the driving force for research of the experimental work of D. Maneerojpakdee: In this context she regrets that she had no time to apply F-CAD in parallel during her stay in Basel, especially as she could have done the same experiments *in silico* and compared the results. In addition, F-CAD is able to predict the effect of the drug particle size and of the shape of the tablet on the dissolution profile, which differs in case of a bi-layer or a coated tablet. In addition, It is also possible to test and calculate the final porosity of the tablet formulation on the release rate. F-CAD needing for the calibration step a minimum of one batch manufactured in the laboratory should allow saving a lot of money for laboratory work. Last, but not least, the findings of this paper may give an incentive to test the benefits of F-CAD by a third party. For the training of future industrial pharmacists in academia and or in an industrial environment it would be of special interest to compare if the same result of the optimal formulation of a 80 mg Nifedipine extended release formulation is obtained and last but not least to compare the costs of this developing project:

- By following strictly the guidelines of ICH Q8 (R2).
- By following the intuition of an experienced formulator (without using experimental design).
- By the application of F-CAD.

The results push forward the idea of adopting the workflow of the automotive and aircraft industry by the pharmaceutical industry: However, only the practical implementation of the workflow of the automotive and aircraft industry will lead to the proof of concept that the application of a virtual formulation tool and the harmonization of the equipment between the R&D and production labs are mandatory to reduce the annual billion dollars of losses due to poor formulations and poor processes.

Impact of the Digital Revolution on the Future of Pharmaceutical Formulation Science

Hans Leuenberger, Michael N. Leuenberger

European Journal of Pharmaceutical Sciences 87 (2016) 100–111

The ongoing digital revolution is no longer limited to the application of apps on the smart phone for daily needs but starts to affect also our professional life in formulation science. The software platform F-CAD (Formulation-Computer Aided Design) of CINCAP can be used to develop and test in silico capsule and tablet formulations. Such an approach allows the pharmaceutical industry to adopt the workflow of the automotive and aircraft industry. Thus, the first prototype of the drug delivery vehicle is prepared virtually by mimicking the composition (particle size distribution of the active drug substance and of the excipients within the tablet) and the process such as direct compression to obtain a defined porosity. The software is based on a cellular automaton (CA) process mimicking the dissolution profile of the capsule or tablet formulation. To take account of the type of

dissolution equipment and all SOPs (Standard Operation Procedures) such as a single punch press tomanufacture the tablet, a calibration of the F-CAD dissolution profile of the virtual tablet is needed. Thus, the virtual tablet becomes a copy of the real tablet. This statement is valid for all tablets manufactured within the same formulation design space. For this reason, it is important to define already for Clinical Phase I the formulation design space and to work only within this formulation design space consisting of the composition and the processes during all the Clinical Phases. Thus, it is not recommended to start with a simple capsule formulation as service dosage form and to change later to a market ready tablet formulation. The availability of F-CAD is a necessary, but not a sufficient condition to implement the workflow of the automotive and aircraft industry for developing and testing drug delivery vehicles. For a successful implementation of the new workflow, a harmonization of the equipment and the processes between the development and manufacturing departments is a must. In this context, the clinical samples for Clinical Phases I and II should be prepared with amechanical simulator of the high-speed rotary press used for large batches for Clinical Phases III & IV. If not, the problem of working practically and virtually in different formulation design spaces will remain causing worldwide annually billion of $ losses according to the study of Benson and MacCabe. The harmonization of equipment and processes needs a close cooperation between the industrial pharmacist and the pharmaceutical engineer. In addition, Virtual Equipment Simulators (VESs) of small and large scale equipment for training and computer assisted scale-up would be desirable. A lean and intelligent management information and documentation systemwill improve the connectivity between the different work stations. Thus, in future, it may be possible to rent at low costs F-CAD as an IT (Information Technology) platform based on a cloud computing solution. By the adoption of the workflow of the automotive and aircraft industry significant savings, a reduced time to market, a lower attrition rate, and amuch higher quality of the final marketed dosage form can be achieved.

Conclusions - Next Steps

The full implementation of the newworkflow of the automotive and aircraft industry for small API molecules and the harmonization of the processes/equipment for eliminating the problems of the industrialization process as a critical path, will need a decision at the top pharmamanagement similar to the decision to bring biologics to the market following the Biotec Revolution. A special working party needs to study carefully the needs for introducing successfully the workflow of the automotive and aircraft industry. This task includes the evaluation and validation of the F-CAD software platform, to establish a decision tree for selecting the appropriate formulation design space according to the results of preformulation studies. The formulation design space for manufacturing samples for Clinical Phases I–III needs to cover in-silico and laboratory validation experiments, which is anyhow a prerequisite. Last but not least this study has to put a special emphasis on the harmonization of processes and of the equipment to avoid subsequent scale-up problems. As an important spin-off of this study an intelligent and lean IT management information/documentation systemwill result,whichwill facilitate the industrialization process from Clinical Phase I to registration.

Development of Desiccant Materials for Cooling Systems Applications, Modeling of Sorption Processes & Experimental Testing of Material Performance

by William M. Worek, Member EUAS

Short Biography

EDUCATIONAL BACKGROUND

- *Ph.D. Mechanical and Aerospace Engineering, Illinois Institute of Technology, 1980.*
- *M.S. Mechanical and Aerospace Engineering, Illinois Institute of Technology, 1977.*
- *B.S. High Honors, Mechanical Engineering, Illinois Institute of Technology, 1976.*

ADMINISTRATIVE EXPERIENCE

- *November 2017 – present*
  Professor, Mechanical and Industrial Engineering, Texas A&M – Kingsville.
- *January 2016 – October 2017*
  Executive Director, Eagle Ford Center for Research Education and Outreach and Professor, Mechanical Engineering, Texas A&M – Kingsville.
- *September 2013 – December 2105*
  Professor and Associate Dean Research and Graduate Studies, Stony Brook University.
- *July 2012 – May 2013*
  Dave House Professor and Dean of Engineering, Michigan Technological University.
- *August 2000 – July 2009*
  Head, Department of Mechanical Engineering, University of Illinois at Chicago.
- *October 2000 – September 2010*
  Director, UIC Industrial Assessment Center, U.S. Department of Energy.
- *August 1999 – July 2000*
  Interim Head, Department of Mechanical Engineering, University of Illinois at Chicago
- *August 1998 – January 2009*
  Director, Energy Resources Center, University of Illinois at Chicago.
- *September 1995 – August 1999*
  Associate Department Head, Department of Mechanical Engineering, University of Illinois at Chicago.

PROFESSIONAL EXPERIENCE

- *August 2013 – preset, Professor, Department of Mechanical Engineering, Stony Brook University.*
- *July 2012 – May 2013, Professor, Department of Mechanical Engineering – Engineering Mechanics, Michigan Technological University.*
- *September 1995 – July 2012, Professor, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *September 1989 – August 1995, Associate Professor (tenured), Department of Mechanical Engineering, University of Illinois at Chicago.*
- *September 1986 – 1989, Associate Professor, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *August 1980 – August 1986, Assistant Professor, Department of Mechanical and Aerospace Engineering, Illinois Institute of Technology.*
- *August 1978 – August 1980, Part–Time Instructor (as a M.S. Graduate Student), Department of Mechanics, Mechanical and Aerospace Engineering, Illinois Institute of Technology.*

- *August 1977 – August 1978, Instructor, Department of Mechanics, Mechanical and Aerospace Engineering, Illinois Institute of Technology.*

UNIVERSITY SERVICE

- *2013 – 2015, Faculty Leadership Team, SUNY – Research Foundation Energy, Environment, Economics, Education (4E) Network of Excellence.*
- *2008 – 2012, Chancellor's Committee on Sustainable and Energy, University of Illinois at Chicago.*
- *2007– 2012, University of Illinois (all campuses), Energy Committee.*
- *2001 – 2002, Academic Leadership Program, One of four UIC members, Committee on Institutional Cooperation, University Memberships include: University of Chicago, University of Illinois, Indiana University, University of Iowa, University of Michigan, Michigan State University, University of Minnesota, Northwestern University, Ohio State University, Pennsylvania State University, Purdue University, University of Wisconsin – Madison.*
- *1995 – 1999, Elected Member, College of Engineering Executive Committee, University of Illinois at Chicago.*
- *1995 – 1997, Chair, Faculty Search Committee, Department of Mechanical Engineering, The University of Illinois at Chicago.*
- *1996 – 1997, Member, Civil and Materials Engineering Department Head Review Committee, College of Engineering, University of Illinois at Chicago.*
- *1995 – 1996, Chair, Chemical Engineering Department Head Search Committee, College of Engineering, University of Illinois at Chicago.*
- *1994 – 1999, Elected Member, Department of Mechanical Engineering Advisory Committee, University of Illinois at Chicago.*
- *1993 – 1994, Chair, College of Engineering Educational Policy Committee, University of Illinois at Chicago.*
- *1993 – 1994, Elected Member, Department of Mechanical Engineering Advisory Committee, University of Illinois at Chicago.*
- *1992 – 1994, Chair, College of Engineering–Nominating Committee for the University Teaching Award, University of Illinois at Chicago.*
- *1989 – 1992, Director of Graduate Studies, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *1989 – 1991, Chair, College of Engineering, Educational Policy Committee, University of Illinois at Chicago.*

RESEARCH INTERESTS

Heat and mass transfer, fluid flow, thermodynamics as applied to energy efficient, renewable and sustainable energy systems. Single and multicomponent absorption and adsorption processes in liquid and solid desiccants, heating and cooling components and systems. Energy policy factors that impact implement of energy systems, energy utilization and energy procurement.

RESEARCH SUPPORT

Professor Worek has received over USD$18M in support of his research. Sponsors have included: U.S. Department of Energy, U.S. Department of Defense, EnergTek, Commonwealth Edison, Tennessee Valley Authority, LaRoche Chemicals, Kaiser Chemicals, the Gas Research Institute, Englehard/ICC, John Crane, Telaire Systems, AEC, Hoechst-Celanese, Oak Ridge National Laboratory, Brookhaven National Laboratory, Ebara Research, Institute of Gas Technology, Munters/Cargocaire, Semco, N-Baro Tech., Blue Moon Fund, and the National Center for Energy Management and Building Technology.

AWARDS

- *Frank Kreith Energy Award, November 2018 (Honoring individuals for significant contributions to a secure energy future with particular emphasis on innovations in conservation and/or renewable energy) – Awarded at the American Society of Mechanical Engineers (ASME) – International Mechanical Engineering Congress and Exhibition (IMECE) Meeting – once per year.*
- *Edwin F. Church Award, 2013 ASME (Established in 1972 to honor individuals for distinguished service to mechanical engineering education in activities other than teaching, research and administration) – Awarded at the ASME IMECE Meeting – once per year.*
- *ASME Distinguished Service Award, 2013.*
- *Fellow, American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE), 2012.*
- *Nominated for UIC Excellence in Teaching Award, 2003 (a UIC Campus-wide Award).*
- *Harold A. Simon Award for Excellence in Teaching, 2000 (a UIC-College of Engineering Award).*
- *Fellow, American Society of Mechanical Engineers (ASME), 2001.*
- *University of Illinois, Committee on Institutional Cooperation (CIC) Academic Leadership Program (ALP) Fellow, 2001–2002.*

Professor Worek's technical area is Mechanical and Aerospace Engineering with expertise in thermal sciences and energy systems. He is an internationally recognized leader in the areas of energy components and systems, and combined single and

multicomponent heat and mass transfer processes. His research, over the last 35 years, has been on the development of desiccant materials for cooling systems applications, modeling of sorption processes, experimental testing of desiccant material performance and the use of desiccant processes in the design and control of cooling, refrigeration and dehumidification systems. These systems are thermally activated making them candidates for activation by solar energy, combined heat and power systems or waste heat utilization. In addition, Prof. Worek and his team were the first to develop the second-law analysis of combined heat and mass transfer processes to evaluate the potential of these systems. He holds three patents on sorption system design improvements and new concepts. Much of this work has published in archival journals and he has given numerous lectures on the subject.

Professor Worek has many other significant accomplishments. He is Co-editor of *Marks' Standard Handbook for Mechanical Engineers*, Co-Editor of the *Handbook of Heat Transfer*. In addition, he is the Editor-in-Chief of the *International Communications in Heat and Mass Transfer*, Executive Editor of *Applied Thermal Engineering*, Coordinating Editor of *Heat Transfer Asian Research* and Associate Technical Editor for *Energy – the International Journal*. Also, he serves on the Editorial Advisory Boards of the *International Journal of Heat and Mass Transfer*, and the *Journal of Power Technologies*. He has chaired the Mechanical and Systems Engineering Board of the Research Grants Council (RGC) of the University Grants Committee (UGC) of Hong Kong. Also, he has made numerous presentations at international conferences and invited presentations worldwide in countries including Brazil, Columbia, China, Japan, the United Kingdom and Italy.

Professor Worek is very active with professional societies in his research area. He is a Fellow of the American Society of Mechanical Engineers (ASME) and he has served as an officer of the ASME – Solar Energy Division, becoming Chair of the Division in 1993 and 1994. He is past Vice-President of ASME's Energy Resources Group, which included the Advanced Energy Systems Division, the Solar Energy Division, the Petroleum Division and the Ocean, and the Offshore and Arctic Engineering Division. Also, he was elected as one of twelve members of ASME's Board of Governors (i.e., ASME's Board of Directors). This prestigious position was for a three-year term that oversaw the overall operation of ASME. In addition, he is a Fellow of the American Society of Heating Refrigerating and Air-Conditioning Engineers (ASHRAE).

Professor Worek's impact on engineering and technical education has been nationally recognized. He is the 2013 recipient of the Edwin F. Church Medal from ASME. The Church Medal is awarded to one person annually at the ASME–IMECE Meeting for seminal contributions to engineering education (see https://www.asme.org/about-asme/get-involved/honors-awards/achievement-awards/edwin-f-church-medal). In addition, he is the 2018 recipient of the Frank Kreith Energy Award. This award honors individuals for significant contributions to a secure energy future with particular emphasis on innovations in conservation and/or renewable energy (seehttps://www.asme.org/about-asme/participate/honors-awards/achievement-awards/frank-kreith-energy-award).

Professor Worek's administrative experience is extensive. At Stony Brook University, he formed a research action team that prepared collaborative proposals, in response to competitive solicitations and corporate needs, in the areas of energy, materials and manufacturing, smart grid, cyber security and advanced computing. The result of those efforts resulted in several multi-institutional programs begin funded.

When Professor Worek was MIE Department Head, he expanded the educational

outreach of the Department. He initiated a new Professional Masters Program, the first in the College of Engineering, which focused on energy. This program, which has been replicated throughout the United States, allowed students with a bachelor's degree to come back to school and receive a master's degree while still working. This effort has been quite successful and continues to be the only such program in the College of Engineering at UIC.

While serving as the MIE Department Head, Professor Worek also was the Director of the Energy Resources Center (ERC), a position that he held for 11 years. The ERC, established in 1973 by the Illinois Board of Higher Education (IBHE), is the only "Energy Center" at the University of Illinois. During his tenure as Director of the ERC, externally funded research increased almost eight times. This funding came mostly from industry.

Also, as ERC Director, Professor Worek formed a Board of Directors that included key industry and agencies in the energy area. These included: Commonwealth Edison, Exelon, Illinois Power, Nicor Gas, Peoples Gas, the Gas Technology Institute, the Electric Power Research Institute, the U.S. Department of Energy-Washington, DC, the Illinois Department of Economic Opportunity, the Chicago Department of the Environment and Argonne National Laboratory.

Representing the University as MIE Department Head and ERC Director, Professor Worek enhanced interaction and outreach with the Illinois Congressional Delegation to promote our research, development and educational programs. He has interacted closely with other energy research institutions. In New York State, these included the Research Foundation for the State University of New York (system wide), SUNY – Buffalo, SUNY – Albany, SUNY – Binghamton, Rochester Institute of Technology, Rensselaer Polytechnic Institute and Syracuse University. In Illinois, Professor Worek interacted with Southern Illinois University, the University of Illinois at Urbana-Champaign, the University of Chicago and Argonne National Laboratory. He represented the University of Illinois at Chicago as a member of the Association of State Energy Research and Technology Transfer Institutes (ASERTTI). ASERTTI membership totals over thirty national organizations, including the California Energy Commission (CEC), the New York State Energy Research and Development Authority (NYSERDA), the Energy Center of Wisconsin, Texas A&M University, Washington State University and the Florida Solar Energy Center (FSEC).

During Professor Worek's tenure as Director, the ERC was recognized by the State of Illinois as "Energy Advisor" to the State. Given this advisory role, he frequently met with State of Illinois decision makers to assist in the formulation of State energy research and development plans, and to assist in implementation of these plans.

In addition, Professor Worek has had long-term technical relationships and collaborations with scientists and administrators United States National Laboratories. These include: Brookhaven National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Argonne National Laboratory. These relationships have been through long-term collaborative projects and consulting.

Professor Worek is quite honored to selected as a member of the EU Academy of Science.

Improvements in Materials and Science Engineering

by Derek O. Northwood, Member EUAS

Short Biography

Professor Derek O. Northwood is a Distinguished University Professor and Professor of Engineering Materials in the Department of Mechanical, Automotive and Materials Engineering at the University of Windsor, Windsor, Ontario, Canada. Professor Northwood has an earned doctorate in Chemical Physics (Crystallography) from the University of Surrey (UK) and a BSc (Eng) in Engineering Metallurgy from the Imperial College, University of London (UK). He is a licensed Professional Engineer in Ontario, Canada (PEng) and is a Chartered Professional Engineer (CPEng; NER), APEC Engineer, and International Professional Engineer (IntPE(AUS), in Australia. In the 40+ years as an academic, Professor Northwood has held various administrative positions including Department Head, Dean, Associate Dean of Research, Director of the Office of Research Services, President of the Industrial Research Institute, and, Research Leadership Chair, both at the University of Windsor and Ryerson University, Toronto, Canada. Professor Northwood has taught, researched and facilitated joint research and educational programs at 14 universities worldwide, including the UK, the USA, Australia, Taiwan, China, Singapore and Canada. He has published 687 papers in refereed international journals and conference proceedings, 9 chapters in books and has edited 7 books, on a wide range of topics including materials and their applications, and engineering and technology education. He has been elected Fellow of five international professional societies in Australia, Canada, the UK and the USA; namely, Fellow of the Royal Society of Canada (FRSC); Fellow of the Institution of Engineers Australia (FIEAust); Fellow of the World Institute for Engineering and Technology Education (FWIETE); Fellow of the Institute of Materials, Minerals and Mining (FIMMM); and Fellow of ASM International (FASM).

SUMMARY OF RESEARCH ACTIVITIES

For nearly 50 years, Professor Derek O. Northwood has built a rich and varied, but consistent, body of work in the broad area of Materials and Science Engineering. Starting from his Ph.D. work at the University of Surrey (UK), and long before it became fashionable to do so, he has always placed his work in the general context of materials processing - structure - properties - performance relationships. The processing-structure-properties-performance (PSPP) tetrahedron is now recognized as the core of Materials Science and is the basis for a "materials by design" approach. Professor Northwood recognized early on in his Ph.D. studies that at the centre of this PSPP tetrahedron was "Materials Characterization" and this has always been the core of Professor Northwood's work.

Professor. Northwood's research work over the years, has examined a wide range of materials and applications. His Ph.D. work studied the effects of ball-milling on ceramic and metallic powders. Today, this work is considered as "Mechanochemistry", a recognized part of chemistry. Research in later years could generally be classified as "Materials for Energy Systems". This included nuclear (zirconium alloys; radiation damage; delayed hydrogen cracking), hydrogen storage, batteries, and fuel cells. In addition to the energy areas, Professor Northwood has contributed greatly to the

understanding of high-temperature deformation (creep) and the degradation of concrete and concrete structures.

The major emphasis of Professor Northwood's research in recent years can be described as "surface engineering". This includes both coatings and other surface treatments including heat treating (carburizing, nitriding, induction heating) and surface patterning. The "coatings" have included nano- and micro-laminated coatings for wear resistance, PVD coatings for stainless-steel bipolar plates, and Plasma Electrolytic Oxidation (PEO) coatings for lightweight alloys (Mg, Al, Ti). Significant advances have been made in understanding the PEO process including the physics of the plasma so as to design coatings with improved corrosion and wear resistance. The citation for Professor Northwood's induction as a Fellow of the Royal Society of Canada in November 2016, read, in part:

"*Dr. Northwood is a world leader in the area of surface engineering, where he is developing novel methods for improving surface properties of different materials.*"

The following is a list of 15 key contributions (papers) over a period of nearly 40 years.

1. D.O. Northwood, Irradiation damage in zirconium and its alloys, Atomic Energy Review, 15(4), 547-610, 1977.
2. D.O. Northwood, R.W. Gilbert, L.E. Bahen, P.M. Kelly, R.G. Blake, A. Jostsons, P.K. Madden, D. Faulkner, W. Bell, R.B. Adamson, Characterization of neutron irradiation damage in zirconium alloys - an international "round-robin" experiment, Journal of Nuclear Materials, 79(2), 379-394, 1979.
3. D.O. Northwood and U. Kosasih, Hydrides and delayed hydrogen cracking in zirconium and its alloys, International Metals Reviews, 28(2), 92-121, 1983.
4. D.G. Ivey and D.O. Northwood, Storing energy in metal hydrides - a review of the physical metallurgy, Journal of Materials Science, 18(2), 321-347, 1983.
5. L. Shi and D.O. Northwood, Strain hardening and recovery during the creep of pure polycrystalline magnesium, Acta Metallurgica et Materialia, 42(3), 871-877, 1994.
6. Z.N. Farhat, Y. Ding, D.O. Northwood and A.T. Alpas, Effect of friction and wear of nanocrystalline aluminum, Materials Science and Engineering A, 206(2), 302-313, 1996.
7. D.O. Northwood and K. Dosen, A metallographic study of abnormal grain growth during aging of a beta-quenched Zr-1-1wt%C-0.08wt%Fe alloy (Reprinted from Metallography, vol 13, pg 249-266, 1980), Materials Characterization, 39(2-5), 381-398, 1997.
8. S.K. Roy, K.B. Poh and D.O. Northwood, Durability of concrete - accelerated carbonation and weathering studies, Building and Environment, 34(5), 597-606, 1999.
9. F. Feng, J. Han, M. Geng and D.O. Northwood, Study of metal hydride electrodes using a novel electrochemical method, Journal of Electroanalytical Chemistry, 487(2), 111-119, 2000.
10. F. Feng, M. Geng and D.O. Northwood, Electrochemical behaviour of intermetallic-based metal hydrides used in Ni/metal hydride (MH) batteries: A review, International Journal of Hydrogen Energy, 26(7), 725-734, 2001.
11. H. Niu and D.O. Northwood, Enhanced electrochemical properties of ball-milled Mg Ni electrodes, International Journal of Hydrogen Energy, 27(1), 69-77, 2002.
12. E. Gyenge, M. Atwan and D. Northwood, Electrocatalysis of borohydride oxidation on colloidal Pt and Pt-alloys (Pt-Ir, Pt-Ni, and Pt-Au) and application for direct borohydride fuel cell anodes, Journal of the Electrochemical Society, 153(1), A150-A156, 2006.
13. Y. Wang and D.O. Northwood, An investigation into TiN-coated316L stainless steel as a bipolar plate material for PEM fuel cells, Journal of Power Sources, 165(1), 293-298, 2007.
14. R.O. Hussein, X. Nie, D.O. Northwood, A. Yeroknin and A. Matthews, Spectroscopic study of electrolytic plasma and discharging behaviour during the plasma electrolytic oxidation (PEO) process, Journal of Physics D: Applied Physics, 43(10), Article number 105203, 2010.
15. A.S. Toloei, V. Stoilov and D.O. Northwood, A new approach to combating corrosion of metallic materials, Applied Surface Science, 284, 242-247, 2013.

As well as the "materials" work, Professor Northwood has made significant contributions to engineering education. The first contribution was a series of four modules for the Journal of Educational Modules for Materials Science and Engineering (now Journal of Materials Education) in 1982 which outlined the theory of x-ray line profile analysis, and described the method's application to the characterization of a wide range of

materials including amorphous materials and polymers. This set of modules contained what are now described as "learning outcomes", long before learning outcomes became part of curriculum design. Professor Northwood's other major contributions to engineering education have been in the areas of "Women in Engineering", including recruitment and retention; "experiential learning", including work-based learning (WBL); problem-based learning (PBL), and co-operative education; and, the liberal education of a holistic generation of engineer, namely, graduates with the skills to work across intellectual, social, and cultural boundaries.

RESEARCH ACTIVITIES & PUBLICATIONS IN 2017/2018 PERIOD

The activities and publications are divided into two primary areas, namely:

1. Developing the potential properties of traditional materials

This is co-operative work with Professor Cheng Liu, College of Mechanical Engineering, Yangzhou University, Yangzhou, China. In this work we have demonstrated how the application of novel processing technologies to traditional materials, such as medium carbon steels and cast irons (ADI), can produce a synergistic multi-phase strengthening effect. One of the strengthening phases is nano super bainite. Example publications include:

Cui, X.[a] , Northwood, D.O.[b] , Liu, C.[a]
Role of Prior Martensite in a 2.0 GPa Multiple Phase Steel
(2018) *Steel Research International*, 89 (10), art. no. 1800207, .
DOI: 10.1002/srin.201800207
[a] College of Mechanical Engineering, Yangzhou University, 196 Huayang Road, Yangzhou, 225127, China
[b] Department of Mechanical, Automotive and Materials Engineering, University of Windsor, 401 Sunset Avenue, Windsor, ON N9B 3P4, Canada

Abstract
A 55Mn2SiCr steel is developed by a novel multiple-step process, which involves austenitizing at 900 °C for 30 min, rapid quenching to 210 °C, then holding at 170 °C for 5 min, and isothermally holding at 250 °C for different times, and finally cooling in air. The mixed microstructure consists of lenticular prior martensite (PM), fine needle bainitic ferrite (BF), and filmy retained austenite (RA). The results show that the highest tensile strength of 2030 MPa with a bending strength of 4000 MPa is achieved at 250 °C for 120 min. This is attributed to a synergistic multi-phase strengthening effect. The presence of martensite formed during the quenching process prior to the isothermal treatment, accelerates the kinetics of subsequent nano-scaled super bainitic transformation by bainitic laths nucleating quickly at the martensite-austenite interfaces. The product of austenite fraction and its carbon content is found to be another important factor for controlling the strength. In addition, the phase evolution as well as carbon partitioning mechanism during isothermal treatment is discussed.

Zhao, E.J.[a] , Liu, C.[b] , Northwood, D.O.[c]
Accelerated Nano Super Bainite in Ductile Iron
(2018) *MRS Advances*, 3 (45-46), pp. 2789-2794. Cited 1 time.
DOI: 10.1557/adv.2018.440
[a] Beijing New Oriental Foreign Language School at Yangzhou, Yangzhou Jiangsu, China
[b] College of Mechanical Engineering, Yangzhou University, Yangzhou, Jiangsu, China
[c] Mechanical Auto and Materials Engineering, University of Windsor, Windsor, ON, Canada

Abstract
A commercial unalloyed ductile iron has been developed to produce a multiphase matrix microstructure consisting of lenticular prior martensite, feathery upper bainite and a nano-scaled super bainite of lath bainitic ferrite and carbon-enriched film retained austenite. Multi-step heat treatment composed of austenizing, rapidly quenching and isothermally holding at low temperature have been developed. A tensile strength of more than 1.6 GPa, a hardness higher than HRC 54, and an elongation in excess of 5%, are achieved. This is attributed to a synergistic multi-phase strengthening effect. The developed nano super bainite exhibits a good balance between strength and toughness. The presence of martensite formed during the quenching prior to the isothermal treatment, accelerates the kinetics of subsequent nano super bainitic transformation by bainitic laths nucleating quickly at the martensite-austenite interfaces.

Liang, Z.[a] , Zhou, W.[a] , Wang, X.[a] , Northwood, D.O.[b] , Liu, C.[a]

A 2.1 GPA triple-phase spring steel
(2018) *WIT Transactions on the Built Environment*, 175, pp. 1-7.
DOI: 10.2495/HPSM180011
[a] College of Mechanical Engineering, Yangzhou University, China
[b] Mechanical, Auto and Mat, erials Engineering, University of Windsor, Canada

Abstract
The key way of achieving sustainability of a product is to design a manufacturing process that increases the mechanical properties of traditional materials, e.g. steel, whilst also increasing processing efficiency, and diminishing energy consumption. A novel process has been developed that allows for a traditional spring steel (60Si2Mn) to be produced with a high level of strength (tensile strength is over 2100 MPa, bending strength is 4100 MPa, yield strength is 1700 MPa as well as hardness of 59 HRC), also retaining reasonable ductility on an industrial scale. It is shown that a triple-phase microstructure comprising lenticular prior martensite, nano-scaled needle/lath-like bainitic ferrite and film retained austenite, is obtained. The excellent combination of strength and ductility is attributed to a synergistic multi-phase strengthening effect. The nano-scaled structure exhibits a good balance between strength and toughness. The presence of prior martensite provides the kinetics of subsequent nano-scaled bainitic transformation by bainitic laths nucleating at the martensite–austenite interfaces. This design methodology potentially broadens the application of spring steel to components that experience more demanding service environments, such as heavy loads.

Liu, C.[a] , Yang, C.[a] , Yuan, L.[b] , Northwood, D.O.[c]
Role of pre-formed martensite on transformation of austempered ductile iron
(2017) *Materials Science and Technology (United Kingdom)*, 33 (15), pp. 1819-1828. Cited 5 times.
DOI: 10.1080/02670836.2017.1323166
[a] College of Mechanical Engineering, Yangzhou University, Yangzhou, Jiangsu, China
[b] Testing Center, Yangzhou University, Yangzhou, Jiangsu, China
[c] Mechanical, Auto and Materials Engineering, University of Windsor, Windsor, ON, Canada

Abstract
A commercial ductile iron is treated by a novel austempering process to obtain a good combination of strength and ductility. The samples are austenitised at 890°C for 10 min, then quenched into patented quenching liquid, and austempered in an electric furnace at 220°C for 5, 10, 30, 60, 240 and 600 min, respectively, finally air cooled. The bending test and the tensile test are conducted and microstructural features are analysed on the austempered ductile iron. The optimum mechanical property is achieved at 220°C for 240 min. Main reason for high strength and ductility is the formation of a fine structure consisting of multiple phases of pre-formed martensite and lath bainitic ferrite with film retained austenite.

2. Innovations in Engineering Education

I have been working with Dr. Daniela Pusca, University of Windsor on innovations that have been incorporated into a first year foundation course in Engineering Design. These innovations include: implementation of the design thinking paradigm; solution focused thinking; implementation of high-impact practices; teaching for creativity; integrative learning; transformative learning; hands-on experiences. Example publications include:

Pusca, D., Northwood, D.O.
Design thinking and its application to problem solving
(2018) *Global Journal of Engineering Education*, 20 (1), pp. 48-53.

University of Windsor, Windsor, ON, Canada

Abstract
In this article, the authors implement the design thinking paradigm as a method to find solutions for specific problems and challenges within higher education. This approach was triggered by the continuous changes in technology and the requirements of the outcome-based curriculum in regard to graduate attributes. The authors also address the question as to whether researchers should be problem focused or solution focused in the process. Problem-oriented thinking is closely linked to critical thinking, and questions like what? and why?, whereas solution-focused thinking is linked to creativity and the question how. In this context, design thinking should be thought as a form of solution-based thinking, which is implemented to produce creative future results and/or creative resolutions to wicked problems. This article identifies how design thinking was implemented to provide innovations in outcome-based teaching and learning considering aspects, such us curricula, pedagogy, assessment methods and teaching spaces. The main goal was to improve graduate attributes and, as a consequence, the academy to industry transition. Using case studies to accommodate the new generation of learners, the authors argue in the article that user-oriented and outcome-based oriented design thinking is the suitable paradigm to ensure that these initiatives are successful.

Pusca, D., Northwood, D.O.
Implementation of high-impact practices in engineering design courses
(2018) *World Transactions on Engineering and Technology Education*, 16 (2), pp. 108-114.

University of Windsor, Windsor, ON, Canada

Abstract
Teaching and learning practices have an impact on students' performance and their ability to achieve the required graduate attributes. Educational institutions are asked to consider practices that ensure both academic success in university and post-graduation outcomes in the workforce. As part of the institutional approach to innovation in teaching and learning excellence, engineering design courses were redesigned to improve student experience, and also to include more high-impact practices. This article examines the high-impact curricular practices that were implemented in engineering design courses as teaching practices, and how they relate to the desired learning outcomes. Student engagement is considered as a measure of effective learning. Using evidence, the authors argue that experiential learning and high-impact practices lead to greater engagement, better prepare students for future employment, and help to bridge acknowledged gaps between education and practice.

Pusca, D.[a] , Northwood, D.O.[b]
Curiosity, creativity and engineering education
(2018) *Global Journal of Engineering Education*, 20 (3), pp. 152-158.

[a] Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada
[b] Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada

Abstract
It has been stated that the need to know is an engine of discovery that motivates humanity to explore, experiment and achieve (Mario Livio and Robin Tatu). In this article, the authors discuss different opinions and definitions associated with curiosity as the need to know, its relation to creativity and the implication for the models of active learning. The purpose is twofold: 1) to better understand why curiosity, as a powerful human force for intellectual and creative expression, motivates stronger student engagement to find solutions for open-ended, complex problems; and 2) to analyse if curiosity and creativity can be cultivated, supported and encouraged or if they are suppressed by person-centred and context-centred factors or the education system itself. Instructors, when reflecting on what and how we teach, must place equal consideration on teaching creatively and teaching for creativity (Sir Ken Robinson). Case studies discuss the role of curiosity and creativity in engineering design courses at the University of Windsor and the instructor's role in creating an engaging, stimulating teaching and learning environment that encourages curiosity, creativity and intellectual dexterity.

Pusca, D., Northwood, D.O.
The why, what and how of teaching: An engineering design perspective
(2017) *Global Journal of Engineering Education*, 19 (2), pp. 106-111.

University of Windsor, Windsor, ON, Canada

Abstract
The why, what and how of teaching are examined from the perspective of teaching engineering design in an integrative learning environment. Why is the guiding vision and relates to why one reads or studies particular topics. It is the starting point of the learning process. Once why has been established, a backward design approach is utilized to formulate the what and how. What relates to the development of discipline-specific skills and competencies. The what for engineering design is considered from the perspective of the ability to a) generate new design solutions; b)improve existing design solutions; and c) manage design. How is the creative strategy that effectively supports transformative learning and can involve three other ways; namely, who, when and where. Successful engineering design education requires the active participation of students in all stages of the educational process.

Pusca, D., Bowers, R.J., Northwood, D.O.
Hands-on experiences in engineering classes: The need, the implementation and the results
(2017) *World Transactions on Engineering and Technology Education*, 15 (1), pp. 12-18.

University of Windsor, Windsor, ON, Canada

Abstract
The mission and vision of engineering education should continuously change its focus to satisfy customers' requirements - the industry and the students as future employees. The main issue that needs to be addressed by faculty that teach undergraduate engineering courses is how well the graduate engineers are equipped with the practical skills required by industry. This article describes a systematic approach for introducing practical hands-on experiences in engineering courses. The case studies illustrate the implementation, the benefits and the results of this approach designed for student engagement. They will demonstrate the importance of considering both virtual materials and physical materials for hands-on activities, and to implement experiential activities that are employed by practicing engineers.

Advanced Metallic and Intermetallic Materials

by Guang Chen, Member EUAS

Short Biography

Prof. Guang Chen is currently a distinguished professor at Nanjing University of Science and Technology, China. He is well known internationally for his outstanding contributions to the design and development of advanced metallic and intermetallic materials. He did pioneer work on deriving new theories of controlling crystallographic orientation based on interfacial anisotropy, developing a new preparation technique with the combination of directional solidification and directional solid-state phase transformation, and mechanistically solving the intrinsic brittleness of bulk metallic glass via introducing in-situ spherical crystalline phases. All his innovative research has significantly promoted the development of structural materials with superior mechanical and metallurgical properties for engineering applications. He has published more than 200 technical papers in archival journals, textbooks, and encyclopedia chapters. His papers have been highly cited by the materials community. He has received numerous honors and recognitions from academia, government, industry, and professional societies, including special allowance of the State Council in 2018, the State Innovation Pioneer Award in 2017, the State Technological Invention Award in 2016, the State Innovative Achievements Award of Industry-University-Research Institute Collaboration in 2014, two Ministry of Education Technological Invention Awards in 1997 and 2012, the Jiangsu Province Patent Inventor Award in 2018, six Province Scientific and Technological Awards in 1995, 2002, 2006, 2007, 2010 and 2013, the Distinguished Award of the 9th International Workshop on Advanced Materials (IWAM) in 2016, and many other awards and citations from state ministries, province government agencies, and Nanjing University of Science and Technology.

Major Achievements and Activities

Prof. Chen has been recognized as a world authority in the field of TiAl intermetallics. His pioneer work on the γ'-Ni_3Al precipitated superalloys during his Ph. D study greatly stimulated his interest in ordered intermetallic alloys. TiAl intermetallics are the only lightweight metallic materials that can serve in oxidative environment at temperature $>$ 600℃ for long time, but their low tensile ductility at ambient temperature severely limits their application. Inspired by the wide application of single-crystal superalloys in turbine engines, he began to study the directional solidification of TiAl single crystals. His innovative research has broken the common knowledge that the lamellar orientation of β-solidification TiAl is uncontrollable due to Burger's relationship. He derived a new theory to control the crystallographic orientation of fully-lamellar TiAl single crystals based on interfacial anisotropy. He successfully prepared well-aligned TiAl single crystals with parallel orientation via the combination of directional solidification and directional solid-state phase transformation. Such single crystals have an excellent combination of superior

strength, ductility and creep resistance. The tensile ductility at room temperature is increased from <2% to 6.9%. The service temperature is increased from ~650℃ to 950℃ (Figure 1). The minimum creep rate and lifetime at 900℃ are 1~2 order of magnitude better than the commercial TiAl-4822 alloy. This distinguished work "polysynthetic twinned TiAl single crystals for high-temperature applications" has been selected as a cover paper in Nature Materials, 15(8)(2016): 876-881, which has been listed as the top 1% papers with high citations by ESI (Essential Science Indicators).

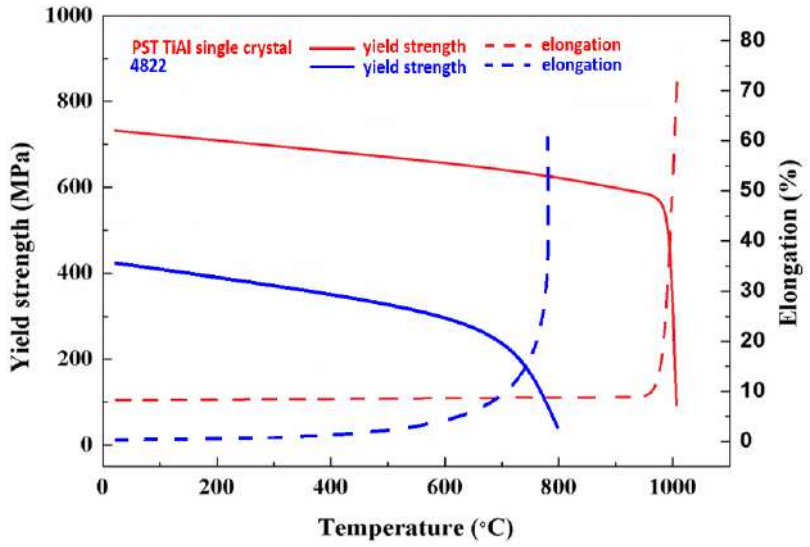

Figure 1. Comparison of tensile properties of polysynthetic twinned (PST) TiAl single crystals and commercial TiAl-4822 alloys

Prof. Chen has also devoted much of his effort to bulk metallic glasses (BMGs). BMGs with an amorphous structure possess many unusual structural and functional properties, but their limited glass forming ability and room temperature brittleness have restricted their further application. He discovered that coarse and spherical in-situ crystalline phases could effectively prevent the propagation of shear bands and promote the ductility of BMGs at ambient temperature (Figure 2), which has been proposed as one of two basic principles of preparing ductile BMGs. He invented semi-solid progressive solidification (SSPS) to eliminate solidification defects and successfully fabricated large-sized Zr-BMG composites with a high tensile ductility (>6%) at room temperature. He also invested the oxygen segregation and proposed a new idea of changing the harmful oxygen embrittlement into solid-solution strengthening, which opens a new window to fabricate ductile BMG composites with low purity of raw materials and low vacuum degree. This distinguished work was included in *The World of Bulk Metallic Glasses and Their Composites*, Research Signpost. It was also granted with the State Technological Invention Award in 2016.

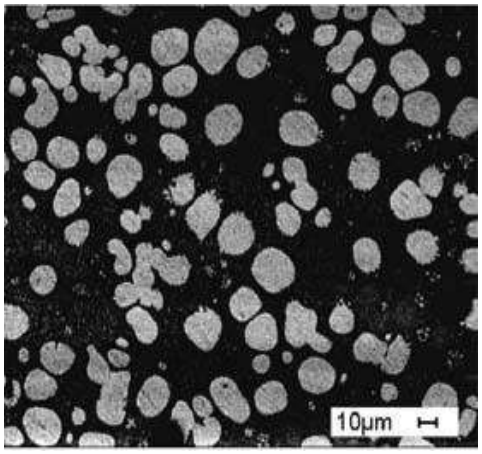

Figure 2. Spherical particles homogeneously dispersed in a metallic glass matrix

Prof. Chen has worked on melt heat treatments during his early career. He proposed that the melt heat treatment changes the melt structure and the liquid-solid interfacial stability, thus realizing the evolution of planar-cellular-dendritic interfaces, which had been confirmed in Sb-Bi alloys, Al-Cu alloys and nickel-based superalloys. The DD98 superalloy single crystals with the melt heat treatment possess 52% finer spacing of primary dendrites. The creep lifetime at 1010℃/248MPa is boosted 1.9 times longer to 107 hours. In recent years, Prof. Chen also focused on the research of nano-precipitated steels. He combined multi-element micro-alloying, ultra-fine grains and nano-precipitation, thus successfully solving the confliction among strength, ductility, corrosion resistance and welding property of low-carbon steels.

Prof. Chen has been granted a total of 62 patents for his innovative work on the development of advanced metallic and intermetallic materials. He was granted the 16th and 19th China Excellent Patent Award in 2014 and 2017. He won the China Invention and Entrepreneurship Award in 2016. He is a member of The Minerals, Metals and Materials Society (TMS), and an associate chairman of Solidification Science and Technology Branch of Chinese Materials Research Society. He is a guest editor of International Journal of *Intermetallics*. He was a chairman of the 6th and 9th International Workshop on Advanced Intermetallic and Metallic Materials. Since 2000, Prof. Chen has mentored over 30 doctors.

Effects of Wind on High- & Low-Rise Buildings

by Qiu-Sheng Li, Member EUAS

Short Biography

Prof. Qiu-Sheng Li is Chair Professor of Civil Engineering and Director of Architecture and Civil Engineering Research Center at City University of Hong Kong. He graduated from Shanghai Jiao-Tong University with BEng in 1984 and from Harbin Institute of Technology with MEng in 1987. He obtained his PhD and the best PhD thesis award (Professor K.H. Hunt Medal) from Faculty of Engineering at Monash University, Australia. Before joining City University of Hong Kong in 1996, Prof. Li had seven years of working experience as a research engineer at Kajima Corporation in Japan and as a consulting engineer in MEL Consultants in Australia. During this period, he was involved in numerous wind engineering and structural dynamic studies on major building and structural developments in Asia and Pacific region. His main research interests and technical expertise are in wind engineering, industrial aerodynamics, engineering mechanics, structural dynamics, and computational mechanics. Over the last thirty years, his research in these fields has resulted in 280 refereed international journal papers and 4 books. Most of the journals are within the top 30% ranking in their respective disciplines according to their impact factors. ***Prof. Qiusheng Li is one of the most cited researchers in civil engineering*** *according to Shanghai Ranking's Global Ranking of Academic Subjects 2016 by Elsevier. Prof. Li has received several awards and honours for his outstanding research contributions including National Natural Science Foundation of Chinese Outstanding Oversea Scientist Award, 2004 and The First Class Award of the Scientific and Technological Progress from the Ministry of Education of China, 2010. He was appointed as Cheung Kong Chair Professor by the State Education Ministry of China and Li Ka Shing Foundation, Hong Kong in 2007 and National Expert of the 1000 Talent Scheme by the Ministry of Human Resources of China in 2013, respectively.* ***In particular, Prof. Li is the recipient of the 2016 Jack E. Cermak Medal from American Society of Civil Engineers (ASCE) in recognition of "his many contributions to wind engineering that range from fundamental to applied research" and "his contributions to structural dynamics studies on major building developments in Asia and the Pacific region".*** *Currently, he is an associate editor of Journal of Structural Engineering, ASCE and an editorial board member of sixteen international journals. Prof. Li has been a principal investigator for over 65 research grants with a total funding over HK$50 million in recent years.*

MAJOR ACHIEVEMENTS AND ACTIVITIES

Prof. Qiu-sheng Li and his research team have been conducting the field measurement of the effects of wind on high-rise buildings and low-rise buildings since 1996. More than ten super-tall buildings—including Shenzhen Pin An Financial Center (600 m high), Taipei 101 Tower (508 m), HK 2 IFC (420 m), Guangzhou West Tower (432 m), Shenzhen Di-

Wang Tower (384 m), and Guangzhou CITIC Plaza (391 m)—have been instrumented through installation of the developed wind and structural health monitoring systems with eight granted patents. **This field measurement program is currently the largest full-scale experiment in the world for studying the effects of wind on high-rise buildings**, which was introduced on the National Geographic Channel and the Discovery Channel as applications of innovative research works. Prof. Li's team has also been carrying out long-term observational study of atmospheric boundary layer wind structure and characteristics over different terrains during tropic cyclones, monsoons and thunderstorms by multi-instruments in Hong Kong and mainland China. The research findings enhanced our understanding of atmospheric boundary layer wind structure and wind effects on high-rise buildings, and also provided valuable information to improve codes of practice such as the suggested design damping values for super-tall buildings and proposed profiles of wind speed, spectra and gust factor for typhoon, monsoon and thunderstorm winds over different types of terrain, which are of importance for the wind-resistant design of high-rise buildings not only in Hong Kong but also in other regions of the world where typhoon or hurricane winds control the design parameters.

Due to most of buildings' damages during windstorms happened on low-rise buildings, Prof. Li's team built and instrumented three full-scale low-rise buildings in the coastal region of South China, a typhoon-prone region for investigating the wind effects on low-rise buildings during extreme windstorms. Since the operation of the program in 2006, monitoring of the wind effects on the three instrumented buildings have been performed during more than twenty tropical cyclones, in particular Severe Typhoon Hagupit and Super Typhoon Rammasun with maximum near-ground wind speeds exceeding 60 m/s captured by the measurement stations. This was perhaps the first time in the field of wind engineering to record the wind effects on low-rise buildings during the passages of extreme wind events. Such information is scarce and vary valuable. The damage mechanisms of building's roofs and claddings caused by strong typhoons were clarified and relevant design guidelines were thus proposed for reduction of typhoon wind damages to residential buildings. The measurements and research findings furthered the understanding of the effects of typhoons on low-rise buildings and advanced the current state of wind engineering.

Prof. Li has made a series of groundbreaking achievements in the field of computational wind engineering (CWE), including a general inflow turbulence generator for accurate simulation of turbulent inlet boundary condition, a new dynamic subgrid-scale model suitable for unstructured or hybrid grids, an efficient method for fluid-structure interaction for turbulent flows with high Reynolds number. In particular, a new simulation approach for evaluation of wind-driven rain (WDR) was proposed based on modified Eulerian multiphase model, which can greatly reduce complexity in evaluations of WDR results and simplifies boundary condition treatments. These research achievements significantly promoted the development of CWE and the practical application of computational fluid dynamics in wind engineering.

In fundamental contribution to wind engineering, Prof. Li carried out a series of wind tunnel studies into the effects of turbulence on pressure fluctuations in separated and reattaching flows. The experiments were conducted in turbulent flows over a much larger range of turbulence length scale than previously studied to explore the mechanisms of the generation of extreme suctions on bluff bodies under flow separation or conical vortex. His research works greatly enhanced the understanding of the effects of turbulence on bluff body aerodynamics.

Prof. Li and his collaborators have also carried out research works on bridge

aerodynamics. The influence of wind characteristics on the aerodynamic admittances and cross-correlation characteristics of buffeting forces for bridge girders with different sections were investigated through a series of wind tunnel tests, which contributed much to the improvement of the buffeting analysis theory. Their investigation on the coupled vibration of galloping and vortex induced vibration of square bridge towers was conducted and the associated mechanisms were explored, and effective vibration suppression measures were proposed. The vortex induced vibration mechanism of central slotted box girder was studied and the suppression measures were presented, which provided valuable guidelines for the wind-resistant design of super long-span bridges. The aerodynamic loads and wind-induced responses of a number of long-span bridges were investigated by field measurements and wind tunnel tests, which ensured the safe design and construction of these wind-sensitive structures.

Besides Prof. Li's research achievements mentioned above, he has also made significant and sustained contributions to professional practice in wind engineering, structural dynamics, structural health monitoring, and wind environment with over 30 year experience as an engineering consultant. His team has undertaken the wind-resistant design or structural health monitoring of more than 150 high-rise buildings and long-span structures by wind tunnel testing, numerical simulation and field measurement. In addition, his contribution to wind engineering and structural engineering extends to service on several national and regional committees such as: the Review of the Code of Practice on Wind Effects in Hong Kong 2004 and National Technical Code for Wind-induced Vibration Control of Building Structures.

Apart from Prof. Li's significant contributions to wind engineering and industrial aerodynamics, he has published more than 100 peer-reviewed journal papers on structural mechanics over the past three decades. His representative works include obtained exact solutions for the generalized Euler's stability problem, buckling of multi-step non-uniform columns with an arbitrary number of cracks subjected to concentrated and distributed axial loads, free vibration of non-uniform rods with arbitrary distribution of mass or stiffness, shear plates, flexural-shear plates with varying cross-section and multi-step orthotropic shear plates, free and forced vibrations of SDOF systems with non-periodically time varying parameters.

In summary, Prof. Li's outstanding achievements made a major impact in advancing the state-of-the-art in atmospheric boundary layer wind characteristics and wind effects on structures through field measurement, wind tunnel testing and numerical simulation. Meanwhile, he has also made significant contributions to the field of structural mechanics.

OUTSTANDING AWARDS

1. Receipt of the 2016 Jack E. Cermak Medal from American Society of Civil Engineers (ASCE) for cumulative distinguished contributions in wind engineering, which is the highest honor in wind engineering, in recognition of "his many contributions to wind engineering that range from fundamental to applied research".
2. Receipt of Lotus (Furong) Outstanding Achievement Award from the Bureau of Education of Hunan Province of the People's Republic of China, 2015.
3. Receipt (Principal Investigator) of the First Class Award of the Scientific and Technological Progress from the Ministry of Education of the People's Republic of China, 2010.
4. Awarded Project Title: Wind Effects on Super-Tall Buildings: Field Monitoring, Wind Tunnel Testing and Numerical Simulation.

5. Receipt (Principal Investigator) of the National Natural Science Foundation of China's Outstanding Oversea Scientist Award, 2004. (Awarded Research Fund: RMB 400,000).
6. Awarded Project Title: Structural Health Monitoring.
7. Receipt of the Second Class Award of the Natural Science from the Ministry of Education of the People's Republic of China, 2004.
8. Awarded Project Title: Wind Resistant Design of High-Rise Structures.
9. The Professor K.H. Hunt Medal Winner in 1997 for Excellence in Research.
10. Awarded Project Title: Turbulence Effects on Bluff Body Aerodynamics.
11. Receipt of the Second Class Award of the Natural Science from the Ministry of Education of the People's Republic of China, 1992.
12. Awarded Project Title: Structural Reliability Theory and Its Application.

HONOURS

1. Member of the EU Academy of Sciences, 2017.
2. Thousand-talent National Expert Professor Appointed by the Ministry of Human Resources of the People's Republic of China, 2013.
3. Chang Jiang (Cheung Kong) Chair Professor Appointed by the Ministry of Education of the People's Republic of China and Li Ka Shing Foundation, Hong Kong, 2007.
4. Lotus (Furong) Chair Professor Appointed by the Bureau of Education of Hunan Province of the People's Republic of China, 2011.

Importance Measures in Reliability, Risk and Optimization

by Way Kuo, Member EUAS

Short Biography

Professor Way Kuo is President of City University of Hong Kong. Before he came to Hong Kong in 2008, he served on the senior management team at the Oak Ridge National Laboratory and as the Dean of Engineering at the University of Tennessee, Knoxville.

Before joining CityU, Professor Kuo was Dean of Engineering at the University of Tennessee and Head of the Department of Industrial Engineering at Texas A&M University. He received his PhD in engineering in 1980 from Kansas State University, and BS in nuclear engineering in 1972 from National Tsing Hua University,Taiwan.

In addition to being a member of the US National Academy of Engineering, he is a foreign member of the Chinese Academy of Engineering, a foreign member of the Russian Academy of Engineering, and a member of Academia Sinica in Taiwan. He is a pioneer in designing and modelling the reliability of electronics systems at the infant stage, renowned for his work on designing reliability in electronics systems. He is the author and co-author of ten academic books and over 200 high impact papers, some of which are deemed classics in systems optimisation design and are used as the basis for establishing the reliability standards. His book, Importance Measures in Reliability, Risk, and Optimization, published by N.Y.: Wiley, 2012, addresses ways to design and enhance reliability of modern systems.

His first popular science book, Critical Reflections on Nuclear and Renewable Energy, has had an impact since its publication in 2013 by Commonwealth Publishing Group in Taiwan. The book has been translated into English, Japanese, French and Russian and published in Massachusetts, Tokyo, Paris, and Moscow, respectively. His new book on higher education, The Soulware with Higher Education, was simultaneously published in Hong Kong, Taipei and Beijing in 2016 under three different publishing houses.

Professor Kuo is the Chairman of the Gnedenko e-Forum based in Moscow, Russia.

Professor Kuo specialises in design for the reliability of electronics systems and nuclear energy. So, his book *Critical Reflections on Nuclear and Renewable Energy* has been published in Taiwan, Hong Kong, Shanghai, Massachusetts, Tokyo, Paris, Seoul, and Moscow.

He was the first foreign expert to arrive following the Fukushima Nuclear Incident. He argues that a holistic view of energy development is required, one that prioritises the production and use of reliable energy sources over that of polluting and volatile ones. He maps out a policy that encourages and rewards the conservation of energy and efficiency in energy use.

A system normally consists of multiple components, which are not necessarily equally important for the performance of the system. Such a system often needs to be designed, enhanced, or maintained efficiently using limited resources. However, for highly complex systems, it may be too tedious, or not even possible, to develop a formal optimal strategy. In these situations, it is desirable to allocate resources according to how important the components are to the system and to concentrate the resources on the small subset of components that are most important to the system. Thus follows the notion of importance measures of components.

For tackling different problems, the distinct importance measures and the associated algorithms should be appropriately designed. Various importance measures have been proposed to judge the relative strength of a component in a system with respect to different criteria. As stated in Griffith and Govindarajulu (1985), no single type of importance measure is universal, since different perspectives on the same system can lead to different views about which factors make one component more important than another. A design engineer may think of a component as being more important if a given reliability improvement in it does more to improve systems reliability than the same reliability improvement in another component. In contrast, an engineer may devise a checklist of components for finding the cause of system failure based on his or her assessment of the conditional probability that a particular component has contributed to system failure. The probabilistic interpretation describing the relation of a component to the functioning or failure of the system is different in each case.

Unique Methods for Studying the Human Sympathetic Nervous System

by Murray Esler, Member EUAS

Short Biography

Senior Director, Baker Heart and Diabetes Institute, Melbourne
Adjunct Professor of Medicine, Monash University, Melbourne
Fellow of the Australian Academy of Science
Prof. Esler is a cardiologist and medical scientist, based at the Baker IDI Heart and Diabetes Institute and the Alfred Hospital, Melbourne, Australia. His research interests are:

The human sympathetic nervous system
Stress, and its effects on the heart and blood pressure
Causes and treatment of high blood pressure and heart failure
Neurotransmitters of the human brain

He is the author of more than 450 papers on these topics. Prof Esler's principal research contribution has been the development of isotope dilution methodology to study the human sympathetic nervous system, and the application of this tool in the investigation of the sympathetic neural physiology of circulatory control, aging, exercise and mental stress responses, and the neural pathophysiology of cardiac failure and essential hypertension. His demonstration of a high level of chronic activation of the cardiac sympathetic outflow in patients with heart failure provided the theoretical backdrop for the evaluation of beta-adrenergic blockers in this condition. More recently, his demonstration of activation of the renal sympathetic outflow in essential hypertension was the stimulus for the development of a new treatment for difficult to control patients, radio-frequency ablation of the renal sympathetic nerves with purpose-designed renal artery catheter.

Awards

** Wellcome (Australia) Medal (1989), awarded annually for "the most outstanding biomedical research in Australia"*
** RT Hall Prize (1996), for research in cardiology, awarded annually by the Cardiac Society of Australasia.*
** Ramaciotti Medal (1997), for excellence in biomedical research.*
** Merck Sharpe & Dohme Award of the International Society of Hypertension (2000)*
** Elected a Fellow of the Australian Academy of Science (2002)*
** Hartnett Medal of the Royal Society of the Arts (Australian Division)*
** Centenary Medal (2003) of the Government of Australia*
** Hamdan Award for Medical Research Excellence (Pathophysiology of High Blood Pressure),United Arab Emirates (2006)*
** Order of Australia; AM (2007)*
** Victoria Prize, State Government of Victoria (2009)*
** Eureka Prize for Translational Research 2011 (shared with Markus Schlaich)*
** Bjorn Folkow Award of the European Society of Hypertension 2012*
** Excellence Award of the Council for High Blood Pressure Research of the AHA 2013*
** Louis F Bishop Award and Keynote Lecturer, American College of Cardiology, 2014*
** American Society of Hypertension Keynote Lecturer and Award, 2014*

I am a cardiologist and medical scientist, working in Melbourne. I list my principal research achievements:

- Developing unique and powerful methods for studying the human sympathetic nervous system
- Applying these methods over three decades in the study of integrated sympathetic nervous responses in health and disease, underpinning the emergence of the new discipline of cardiovascular neuroscience
- Delineating the syndrome of neurogenic essential hypertension, in which the sympathetic nervous system initiates and sustains the blood pressure elevation,

with demonstration that activation of the renal sympathetic nerves is of prime importance in hypertension pathogenesis

- Translation of this knowledge on hypertension into medical care, in contributing to the development and clinical testing of a device treatment for severe, drug-resistant hypertension, the catheter-based radiofrequency ablation of the renal nerves

Developing unique methods for studying the human sympathetic nervous system

In the 1970s measurements of the concentration of the sympathetic nervous system transmitter, noradrenaline, in plasma serves as the most commonly used (but very imperfect) method for quantifying human sympathetic nervous responses. Esler developed an isotope dilution method, with radiolabelled noradrenaline (Life Sciences 1979;25:1461-1470), which was a valid technique for studying the sympathetic nervous system by measuring the release rate of the neurotransmitter from the sympathetic nerves. The technique for measuring the overall appearance rate of noradrenaline in plasma, colloquially termed total noradrenaline "spillover", came to be adopted internationally, as illustrated by its use in the April a 1998 studies of neural circulatory control on board Space Shuttle Columbia.

A more instructive method was needed, however, than this global measure of human sympathetic activity. Esler established a technique for measuring organ-specific noradrenaline release to plasma, for studying regional sympathetic nervous function in the heart and kidneys (1). For the first time this provided a valid technique for studying in humans the sympathetic nerves of internal organs. The theory of all this was clear enough, but the logistics were complicated. How could the central venous catheterisation necessary for sampling from the veins draining internal organs receive ethical approval? Here Esler drew on an unusual background, which coupled his clinical experience as a practising cardiologist with his research life as a neuroscientist. The solution was to graft the research study on to a clinically justified procedure. Sampling from the renal veins for renin measurements was common in the clinical evaluation of hypertension at the time, to screen for a functionally significant renal artery stenosis. This provided an opportunity, with appropriate consent, to establish the renal noradrenaline spiller measurement methodology. Clinical right heart catheterisation enabled the coronary venous sinus sinus sampling required for cardiac noradrenaline spillover measurements (1). The new methodology was unveiled at the 1982 Mexico City meeting of the International Society of Hypertension (Clin Sci 1982;63:285S-287S) and the 1983 San Diego meeting of Juvenile Diabetes Foundation International (1).

Application of these methods in the study of integrated sympathetic nervous system responses in health and disease.

Application of the new radiotracer measures of sympathetic nervous activity led to a new understanding of sympathetic neural metabolic and circulatory responses in health, and in sympathetic neural pathophysiology in disease. Sympathetic activation had been envisaged as global and undifferentiated, as proposed by Walter Cannon in his "fight or flight" formulation. Esler's application of regional noradrenalin spillover methodology refuted this idea. In a given situation sympathetic activation in one sympathetic outflow might be accompanied by a decrease or no change in another; this meant that therapeutic antagonism of sympathetic activation in diseases can be *targeted to the offending organ-specific sympathetic outflow.* His demonstration of preferential activation of the cardiac sympathetic outflow in heart failure provided theoretical justification for the evaluation of beta-adrenergic blockers in this condition, and his demonstration of activation of the renal sympathetic outflow in essential hypertension was a stimulus for the development of a revolutionary antihypertensive treatment, catheter-based renal denervation, described in this nomination.

In *cardiac failure*, a direct change in medical practice followed from a better understanding of neural pathophysiology elucidated by the noradrenaline spillover method. In a definitive paper (Circulation 1986;73:615-621) Esler and his PhD student Greg Hasking demonstrated that, despite an earlier misconception that the failing heart was sympathetically denervated, because myocardial content was decreased, the sympathetic nerves were in reality remarkably stimulated. A prospective study in severe heart failure demonstrated that the level of cardiac sympathetic activity was the strongest predictor of death (J Am Coll Cardiol 1995;26:1257-1263). This research program underpinned the subsequent successful testing and introduction of beta-adrenergic blocking drugs for the treatment of heart failure, and was pivotal for the coordinators of the landmark Carvedilol trial. Esler presented his heart failure research findings, by invitation, at the launch of Carvedilol at the 1996 meeting of the American College of Cardiology (Am J Cardiol 1997;80:7L-14L).

Pioneering the discipline of Clinical Cardiovascular Neuroscience

A review by Esler and colleagues (2) provided a synthesis of the findings when this methodology was applied to the field of cardiovascular medicine. This review is regarded by many as the "bible" of cardiovascular neuroscience. The development of this field has been central to advances in the understanding and treatment of hypertension and heart failure.

Delineation of the syndrome of Neurogenic Essential Hypertension

For the past three decades a major focus in high blood pressure research has been the renin-angiotensin system. Despite the historic collaborative study of Esler and Stevo Julius (New Engl J Med 1977;296:405-411) performed in Michigan which pointed to importance of the sympathetic nervous system, the proven value of antihypertensive drugs blocking the renin-angiotensin system deflected hypertension research elsewhere. This was the context in which, against the tide of medical opinion and interest, Esler on his return to Melbourne set out to further study whether essential hypertension could be neurogenic (initiated and sustained by the sympathetic nervous system). As described , first Esler developed a radioisotopic method to measure organ-specific sympathetic transmitter release to plasma, the *regional noradrenaline spillover rate* measurement (1). For the first time this provided a valid technique for studying sympathetic nerves in internal organs in humans. The regional noradrenaline spillover methodology was then applied in untreated patients with essential hypertension. These studies were derivative of the earlier Michigan studies in neural mechanisms of prehypertension, which can be regarded as their progenitor, but with the application of the more incisive methods for studying the sympathetic nervous system.

The findings were clear cut (3). Essential hypertension very commonly was neurogenic! Sympathetic activation in the cardiac and renal sympathetic outflows was the rule at the inception of hypertension in younger patients. A high level of renal sympathetic activation was later demonstrated in most patients with severe, drug-resistant hypertension (Curr Hypertens Rep 2015;17:519-526). In obesity-related hypertension, again renal sympathetic activation was prominent (4), but here the sympathetic activation was regionalized, excluding the heart. Cardiac sympathetic activation is important in pathogenesis of the blood pressure elevation in Prehypertension, in the early hyperdynamic phase characterised by an elevated heart rate and cardiac output (Circulation 1968;38:282-288) which is an antecedent to later phases in hypertension evolution. *The feature common to all established hypertension phenotypes, however, is activation of the renal sympathetic nerves.* Renal sympathetic activation is key in established hypertension pathogenesis by causing renal tubular reabsorption of sodium, secretion of renin and renal vasoconstriction (Am J Physiol 2010;298:R245-R253).

Testing for the presence of molecular stress biomarkers (Clin Exp Pharm Physiol 2008;35:498-502) suggested that the origins of the sympathetic activation in hypertension lies in chronic mental stress exposure. The exposed stress biomarkers in hypertensive patients

included the existence of adrenaline co-release from sympathetic nerves of the heart and the presence of the adrenaline-synthesizing enzyme, PNMT, in sympathetic nerves accessed via subcutaneous vein biopsies. These changes are seen in experimental animals exposed to chronic stress. Additional evidence of stress exposure in essential hypertension patients was the increased noradrenaline turnover in subcortical brain regions detected with internal jugular venous sampling (Hypertension 1992;19:62-69). This evidence for an importance of chronic mental stress in hypertension pathogenesis resonated with the earlier reports from Ann Arbor of suppression of hostility as an operative psychogenic mechanism in mild hypertension (New Engl J Med 1977;296:405-411).

Development and testing of catheter-based radiofrequency ablation of the renal sympathetic nerves as a treatment for essential hypertension

This demonstration of activation of the renal sympathetic outflow in all phenotypes of essential hypertension, coupled with studies of surgical renal denervation in experimental hypertension under pinned the development of a novel device treatment of hypertension, *catheter-based ablation of the renal nerves,* where perivascular sympathetic nerves lying adjacent to the renal arteries are destroyed by delivering high energy radio waves into the renal artery lumen. Esler and his Melbourne colleagues conducted the first, successful trials of renal denervation (5). These positive results were challenged by the influential, negative US regulatory trial, Symplicity HTN-3 (New Engl J Med 2014;370:1393-1401) but this trial is now discredited because of procedural and technical defects (J Am Soc Hypertens 2014;8:593-598; Eur Heart J 2015;36:217-227). Three subsequent positive, sham-controlled renal denervation trials affirm the treatment's efficacy and safety (Lancet 2017;390:2160-2170; Lancet 2018;391:2346-2355; Lancet 2018;391:2355-2365). A second US Pivotal trial has commenced, notably in patients with untreated hypertension, testing renal denervation as an alternative to antihypertensive medication. It has been suggested that, with time, perhaps regrowth of the ablated renal sympathetic nerves may occur, cancelling out the blood pressure benefit, but with follow-up now as long as ten years, it does appear that pressure lowering is permanent. Renal denervation, with which Esler has had close involvement at both theoretical and practical levels, represents a paradigm shift in hypertension treatment.

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2. Esler M, Jennings G, Lambert G, Meredith I, Horne M, Eisenhofer G. Overflow of catecholamine neurotransmitters to the circulation: Source, fate and functions. Physiological Reviews 1990;70:963-985 (citations 886)
3. Esler M, Jennings G, Korner P, Willett I, Dudley F, Hasking G, Anderson W, Lambert G. The assessment of human sympathetic nervous system activity from measurements of norepinephrine turnover. Hypertension 1988;11:3-20 (citations 708)
4. Rumantir MS, Vaz M, Jennings GL, Collier G, Kaye DM, Seals DR, Wiesner GH, Brunner-LaRocca HP, Esler MD. Neural mechanisms in human obesity-related hypertension. Journal of Hypertension 1999;17:1125-1133 (citations 366)
5. Symplicity HTN-2 Investigators (M Esler CI). Renal sympathetic denervation in patients with treatment-resistant hypertension (The Symplicity HTN-2 Trial): a randomized controlled trial. Lancet 2010;376:1903-1309 (citations 2372)

Innovative Developments in Ion-Solid Interactions

by William J. Weber, Member EUAS

Short Biography

Governor's Chair Professor, Department of Materials Science and Engineering, The University of Tennessee - Knoxville

Prof. William J. Weber received his PhD in Nuclear Engineering from the University of Wisconsin - Madison, USA. He joined Pacific Northwest National Laboratory (PNNL) in 1977 as a research scientist and was appointed Laboratory Fellow in 1997. During 1983, he was a visiting scientist at the Institute for Transuranium Elements in Karlsruhe, Germany, He joined the faculty at the University of Tennessee in 2010 as the Governor's Chair Professor for Radiation Effects in Materials, with a joint appointment at Oak Ridge National Laboratory. His research has encompassed the fundamental aspects of radiation-solid interactions, radiation effects in materials, ion beam modification and analysis of materials, and defects and defect processes in materials. Much of his current research emphasizes the coupling of electronic and atomic energy dissipation processes and their role on radiation effects, defect evolution, formation of novel nanostructures, creation of new functionalities, and the response of materials to extreme environments. He is a member of the EU Academy of Sciences (2016), Fellow of the American Ceramic Society (2000), Fellow of the American Association for the Advancement of Science (2006), Fellow of the Materials Research Society (2008), Fellow of the American Physical Society (2010) and Fellow of the Ion Beam Society of India (2016). He is the recipient of the Lee Hsun Lecture Award (2015); the Outstanding Young Alumni Award (1983) and the Distinguished Alumni Award (2009) from the University of Wisconsin - Oshkosh; the PNNL Laboratory Director's Award for Individual Lifetime Achievement in Science & Technology (2009); the PNNL Laboratory Director's Award for Scientific and Engineering Excellence (1995); the PNNL Chester L. Cooper Mentor of the Year Award (2005); and the U.S. Department of Energy's Materials Science Award for Research with Significant Implication for DOE Related Technologies (1995). He has published more than 530 journal articles, 113 peer-reviewed conference papers, and 13 book chapters. Based on the Web of Science, his publications have over 16,500 citations, with an h-index of 61; based on Goggle Scholar, his publications have been cited over 22,800 times, with an h-index of 73.

The interaction of energetic ions with a solid is well known to result in inelastic energy loss to electrons and elastic energy loss to atomic nuclei in the solid. However, the coupled effects of these energy loss pathways and the critical role of energy dissipation processes on defect production and the evolution of defects, nanostructures and phase transformations under far from equilibrium conditions in materials are complex and not well understood. Particularly challenging are the dynamics of energy transfer processes to electrons and the exchange of energy between electrons and the atomic nuclei via electron-phonon coupling. In general, the electrons along the ion path undergo a large degree of

excitation and electron–electron scattering, and they subsequently transfer much of their energy, via electron–phonon coupling, to atoms in the same region, causing a highly-localized thermal spike. This partitioning of energy deposition and energy dissipation on the electronic and atomic structures are important to the control of ion beam modification methods to create defects and nanoscale structures that tailor materials properties or create new functionalities, as well as the development of radiation-tolerant materials and devices. Predicting and modeling such complex processes, which are temporally and spatially coupled, are grand challenges that demand fundamental understanding of materials processes at the level of electrons and atoms over several orders of magnitude in time scale, from femtoseconds to nanoseconds.

Understanding energy dissipation processes in electronic/atomic subsystems and subsequent non-equilibrium defect evolution is a long-standing challenge in materials science. In the intermediate energy regime, energetic particles simultaneously deposit a significant amount of energy to both electronic and atomic subsystems of silicon carbide (SiC). We have demonstrated that defect evolution in SiC closely depends on the electronic-to-nuclear energy loss ratio (S_e/S_n), nuclear stopping powers (dE/dx_{nucl}), electronic stopping powers (dE/dx_{ele}), and the temporal and spatial coupling of electronic and atomic subsystem for energy dissipation. Our integrated experimental and simulation studies reveal that: 1) increasing S_e/S_n slows damage accumulation; 2) the transient temperatures during the ionization-induced thermal spike increase with dE/dx_{ele}, which causes efficient damage annealing along the ion trajectory; 3) for more radially confined displacement damage within the thermal spike, damage production is suppressed due to the coupled electronic and atomic dynamics. Ionization effects are expected to be more significant in materials with covalent/ionic bonding involving predominantly well-localized electrons. Insights into the complex electronic and atomic correlations will pave the way to better control and predict SiC response to extreme energy deposition.

Perovskite structured oxides, such as $SrTiO_3$, $LiTaO_3$ and $KTaO_3$, are considered critical materials in the area of functional oxide electronics, with unexpected and emergent functionalities, as well as for catalysis and photochemistry applications. In $SrTiO_3$, substantial efforts have been devoted to elucidate the role of oxygen vacancies and localized electronic states, such as polarons, on those properties. A new model has been developed that assigns a definitive red luminescence signature at 2.0 eV to Ti^{3+} polarons trapped at isolated oxygen vacancies. This emission provides an unequivocal identification for the oxygen vacancies, which allows monitoring their creation and annealing by a variety of physio-chemical treatments. Ionoluminescence with energetic (MeV) ion beams has enabled such identification by combining the sensitivity and resolution of spectroscopic techniques with their *in-situ* character, as well as controlled incorporation of point defects, such as oxygen vacancies. Alternative models assigning the blue luminescence emission at 2.8 eV to oxygen vacancies are not supported by the experimental results. Therefore, oxygen vacancies *shine red* and *not blue*, as previously proposed.

We have irradiated $SrTiO_3$ over a wide range of ion fluences at room temperature with different ion species in order to deposit different amounts of energy to target electrons and atomic nuclei by varying the ratio of electronic to nuclear energy loss. The results unambiguously show a dramatic difference in behavior of $SrTiO_3$ irradiated with light ions (Ne, O) compared to heavy ions (Ar). While the damage accumulation and amorphization

under Ar ion irradiation are consistent with previous observations and existing models, the damage accumulation under Ne irradiation reveals a quasi-saturation state at a fractional disorder of 0.54 at the damage peak for an ion fluence corresponding to a dose of 0.5 dpa; this is followed by further increases in disorder with increasing ion fluence. In the case of O ion irradiation, the damage accumulation at the damage peak closely follows that for Ne ion irradiation up to a fluence corresponding to a dose of 0.5 dpa, where a quasi-saturation of fractional disorder level occurs at about 0.48; however, in this case, the disorder at the damage peak decreases slightly with further increases in fluence. This behavior is associated with changes in kinetics due to irradiation-enhanced diffusional processes that are dependent on electronic energy loss and the ratio of electronic to nuclear energy dissipation. Damage accumulation in $SrTiO_3$ single crystals, irradiated with 200 keV Ar ions at 16 and 300 K, has also been investigated using Rutherford backscattering spectrometry along the <100> channeling direction. Amorphization at 16 K occurs at a much lower fluence than at 300 K. Based on model fits to the data, only point defects and amorphous pockets are formed under irradiation at 16 K, while point defects, defect clusters and amorphous pockets are formed at 300 K. High defect mobility under irradiation at 300 K tends to promote annealing and clustering of point defects, while defects appear to be relatively immobile at 16 K.

We have investigated the separate and combined effects of electronic and nuclear energy deposition on microstructure evolution in z-cut $LiTaO_3$. Irradiation of pristine $LiTaO_3$ samples with 2 MeV Ta ions leads to amorphization due to the accumulation of irradiation damage, described by a disorder accumulation model. While 21 MeV Si ions do not produce significant damage in pristine $LiTaO_3$, introduction of pre-existing defects sensitizes $LiTaO_3$ to the formation of amorphous ion tracks from the electronic energy loss by 21 MeV Si ions that induce a synergistic two-stage phase transition process. During the first stage, a possible ferroelectric phase transformation occurs that sufficiently changes the electronic structure, which promotes the formation of amorphous tracks by 21 MeV Si ions during the second stage. This synergistic effect could be a promising tool to functionalize materials for optical devices applications by creating novel cylindrical interfaces and nanostructures to functionalize thin film structures, including tunable electronic, ionic, magnetic and optical properties.

Damage production and amorphization in $KTaO_3$ irradiated with noble-gas ions (40 keV He to 480 keV Kr) have been studied using ion channeling measurements. The damage evolution follows a disorder accumulation model, and the cross-sections for direct-impact and defect-stimulated amorphization have been determined. These cross-sections exhibit a strong dependence on the calculated damage cross sections for displacing lattice atoms, indicating a dominant contribution of nuclear collisions to defect production and amorphization processes under these irradiation conditions. These experimental findings, along with the model fits, suggest that the difference in recoil spectra between He ions and the other heavier ions may be the main driving force for the decreased damage efficiency observed for He ions.

The modification of the local structure in cubic perovskite $KTaO_3$ irradiated with 3 MeV and 1.1 GeV Au ions has been studied by Raman and x-ray absorption spectroscopy, complemented by density functional theory (DFT) calculations. In the case of irradiation with 3 MeV Au ions, where displacement cascade processes are dominant, the Ta L_3-edge x-ray absorption measurements indicate that a peak corresponding to the Ta–O bonds in

the TaO_6 octahedra splits, which is attributed to the formation of Ta_K antisite defects that are coupled with oxygen vacancies, V_O. This finding is consistent with the DFT calculations. Under irradiation with 1.1 GeV Au ions, the intense ionization and electronic energy deposition lead to a blue shift and an intensity reduction of active Raman bands. In the case of sequential irradiations with 3 MeV Au ions followed by 1.1 GeV Au ions, extended x-ray absorption fine structure measurements reveal a decrease in concentration of coupled Ta_K-V_O defects compared to irradiation with just 3 MeV Au ions.

The atomically disordered oxides are seen as suitable candidate for fast oxygen conduction due to a remarkable enhancement in oxygen diffusivity as compared to the ordered oxides. In particular, the disordered derivative of pyrochlore structured oxides ($A_2B_2O_7$) is seen as an intriguing prospect due to intrinsic existence of an oxygen vacancy in the lattice. Using energetic ion irradiation, we demonstrate the fabrication of structurally disordered nanoscale channels in $A_2B_2O_7$ (A = Gd, Yb and B = Ti, Zr) that act as selective pathways for fast oxygen conduction. Atomic-level characterization reveals that the amorphous core and surrounding defect-fluorite phase in the nanochannels exhibit distorted and differently coordinated Ti-O polyhedra, with very similar electronic structure. The formation of defect-fluorite structure is facilitated by the decrease in the difference between ionic radii of A- and B-site cations in the lattice.

High Temperature Oxidation & Hot Corrosion Resistant Nanocrystalline Coating

by Fuhui Wang, Member EUAS

Short Biography

Professor, School of Materials Science and Engineering, Northeastern University, Shenyang 110819, China.
President of Chinese Society for Corrosion and Protection (2014-Present)
ACADEMIC QUALIFICATIONS
Ph.D. in Corrosion Science, October 1992
State Key Laboratory for Corrosion and Protection, Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China
MSc in Materials Science, March 1986
Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China
BEng in Materials and Heat-treatment, July 1983
Harbin Engineering University, Harbin, China
PROFESSIONAL EXPERIENCE
April 2016 –Present: Professor of School of Materials Science and Engineering, Northeastern University, Shenyang, China.
July 1999 – March 2016: Chief Professor for corrosion and protection, and Director of State Key Laboratory for Corrosion and Protection, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China. In charge of research activities in the electrochemical corrosion, high temperature corrosion and protection as well as supervision for Ph.D. students. The main research interest focuses on synergistic effect of water vapor and solid NaCl on corrosion of materials at intermediate high temperature (300-600°C), chemical stability of nanostructured materials, corrosion and protection of magnesium alloys and high temperature coatings such as MCrAlY, TiAlN and enamel coatings.
August 1998 – July 1999: Professor and Deputy Director of Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China. Responsible for all research activities of the institute.
September 1996 – July 1998: Professor and assistant Director of Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China, worked on the projects "High temperature corrosion and protection of Ti-Al based intermetallics".
February 1996 –August 1996: Visiting Professor at University of New South Wales, Sydney, Australia, worked on high temperature corrosion of alloys and coatings in CO environment.
September 1994 – January 1996: Professor of Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, and Director of Surface Engineering Laboratory for Young Scientists, Chinese Academy of Sciences, Shenyang, China.
September 1992 – August 1994: Associate Professor of Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China.
August 1989 - September 1992: Ph.D. student at Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China. The dissertation was "High Temperature Nanocrystalline Superalloy Coatings".
October 1990 – September 1991: Visiting student at Technical University of Munich, Munich, Germany.
March 1986 – August 1999: Research assistant at Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences, Shenyang, China.

Brief Introduction of Prof. Fuhui Wang

Prof. Fuhui Wang was born in 1960, received his B.S. degree in Materials Science from the Harbin Engineering University in 1983 and M.S. degree in Materials Science from Institute of Metal Research, Chinese Academy of Sciences in 1986 and Ph.D. degree in Corrosion and Protection from Institute of Corrosion and Protection of Metals, Chinese Academy of Sciences in 1992. Prof. Wang has been a full professor in the Institute of Corrosion and Protection of Metals since 1994 and was deputy Director of the institute from 1998 to 1999. In 1999, he was appointed as the director of the State Key Lab for Corrosion and Protection, Institute of Metal Research, CAS, and as Chairman of High Temperature Committee of Chinese Society for Corrosion and Protection in 2001. Prof. Wang worked in Technical University of Munich, Germany for one year and six months in University of New South Wales, Australia. He was appointed as Editorial Advisory Board member of Anti-Corrosion Methods and Materials and International Journal of Materials and Product Technology, UK and Editor-in-chief of Corrosion Science and Protection Technology, China in 2004. He became the associated editor of NPJ (Nature partner journal) Material degradation in 2016.

His main research interests focus both on fundamental and applied research of corrosion at high temperatures including oxidation and hot corrosion resistant nanocrystalline coatings, synergistic effect of solid NaCl and water vapor on corrosion of materials at intermediate high temperatures (300-600°C), protective coatings for turbine blades such as aluminide, MCrAlY, TiAlN and enamel coatings. He also emphasized on research directions of corrosion and protection of magnesium alloys and organic nano-paints. Prof. Wang have successfully built up collaborations with numerous universities such as Hokkaido University and Osaka University, Japan, Surrey University, UK, Auckland University, New Zealand, University of New South Wales, Australia and Royal Institute of Technology, Sweden. Prof. Wang received Young Scientists and Engineers Award presented by International Union of Materials in 1993 in Japan, Young Expert Title of Outstanding Achievements, CAS in 1994 and Innovation Award of Science and Technology for Young Scientists, CAS in 2001. In 2014, Prof. Wang was elected to be the President of Chinese Society for Corrosion and Protection. In 2016 he transferred to Northeastern University, Shenyang China. So far, he has authored and co-authored more than 400 scientific publications in peer-reviewed journals. He joined Shenyang National laboratory for Materials Science, leading the area of corrosion and protection of materials.

Research Highlights

High temperature oxidation and hot corrosion resistant nanocrystalline coating

Traditional high temperature oxidation and hot corrosion coatings are divided into three types: aluminide or modified aluminide coatings such as Cr-Al, Si-Al and Pt-Al; MCrAlY (M=Fe, Co and/or Ni) overlay coatings and MCrAlY + Y_2O_3/ZrO_2 thermal barrier coatings. The drawback of these coatings is that their compositions are very different from their substrate alloys. Protection comes from the high aluminum content in the coatings to

form Al_2O_3 on the surface at high temperature. However, these coatings may be harmful to the mechanical properties of the alloys as a result of the inter-diffusion or thermal mismatch between coatings and substrates. An innovative coating has been developed: high temperature oxidation and hot corrosion resistant nanocrystalline coating. The main progress made is that the grain size of the coating is several orders of magnitude smaller than that of the substrate. Thus, the formation of protective Al_2O_3 scale is not from the high aluminum content, but the grain boundary diffusion. The main advantage of this novel coating is that neither inter-diffusion nor thermal mismatch exist between coating and substrate. He also proposed that "super-alloys can protect themselves through nano-crystallization". The referee of the invited manuscript "high temperature oxidation and hot corrosion resistant nanocrystalline coating" at 11^{th} International Symposium on Processing and Fabrication of Advanced Materials held at USA in 2002 gave the comments "Deposition of nanocrystalline coatings have the same composition as the substrate alloys by magnetron sputtering is a novel approach to solve the old problems. It may prove to be a new research direction for the development of high temperature protective coatings". The paper was recommended to be published in Surface Engineering, 2003.

Synergistic effect of solid NaCl and water vapor on corrosion of materials at intermediate high temperatures

It is well known that the severe corrosion occurred on the compressor blades in gas turbine engines in marine environments, which operated at temperatures around 300-600^{o}C. This type of corrosion may be induced by the synergistic effect of solid salt deposits and water vapor. However, there has been little systematic study on this problem up to now. We systematically studied the synergistic effect of solid salt deposits and water vapor on corrosion of 1Cr11Ni2W2MV steel, Fe-Cr alloys, high temperature titanium alloy Ti-60, superalloy K38G, and TiN, TiAlN and enamel coatings at 300-600^{o}C. It was found that solid NaCl deposit and water vapor significantly accelerated the corrosion of materials, especially for Fe-Cr alloys, the corrosion rates increased with increasing Cr content. We proposed the mechanism that the kinetic water film existing on the alloy surface, which induced electrochemical corrosion of alloys. Then we suggested to use (TiAl)N and enamel coatings to protect the compressor blades of turbine engines used in marine environments. We published more than 30 peer-reviewed papers including Oxidation of Metals and Corrosion Science.

Structural Health Monitoring Techniques, Vibration Control & Structural Dynamics

by Wiesław Ostachowicz, Member EUAS

Short Biography

Prof Wiesław Ostachowicz was graduated from Gdansk University of Technology, Poland (receiving BSc and MSc degree in Mechanical Engineering). He defended PhD at Gdansk University of Technology, Poland (in Mechanical Engineering), and defended DSc (habilitation, 1980) at Gdansk University of Technology, Poland (in Mechanical Engineering). In 1989 the President of Poland nominated him to the Professor position (Professor Title). Earlier he was recommended to this position by the Institute of Fluid Flow Machinery, Polish Academy of Sciences (IMP PAN). He is the Corresponding Member of Polish Academy of Sciences (elected on December 1, 2016).

Prof W. Ostachowicz was employed in several institutions: (1) in the IMP PAN, Gdansk (1970–1972) as an assistant; (2) in Navy Shipbuilding Yard, Gdynia (1972–1973) as a designer; (3) at Gdansk University of Technology, Department of Mechanical Engineering (1973–1987) as senior assistant, assistant and associate professor; (4) in the IMP PAN (1986–present) as an associate professor and professor (from 1989); (5) in Gdynia Maritime University (2004–2012) as an associate professor and (6) at Warsaw University of Technology (2013–2017) as an associate professor.

The list of his temporary positions opens: chairman of the Department of Mechanics and Strength of Materials at Gdansk University of Technology (1982–1987), the deputy director for scientific affairs at the IMP PAN (1986–1992); head of the Centre for Mechanics and Machines (from 1998– present), at the IMP PAN; and a chairman of the Department of Mechanics of Intelligent Structures (from 1996– present) at the IMP PAN. He was also employed as an expert of UNIDO (United Nations Industrial Development Organization) at the Instituto de Investigaciones Electricas, Cuernavaca, Morelos, Mexico (1987 and 1990). He was Visiting Professor at: (1) the Syracuse University, the Department of Mechanical Engineering, USA (1980–1981); (2) the University of Glasgow, the Department of Mechanical Engineering, UK (2000–2003); (3) the University of Northampton, the School of Science and Technology, UK (2014–2016); (4) Ecole Nationale Supérieure d'Arts et Métiers (ENSAM), Paris, France (2017).

Prof W. Ostachowicz has led dynamics research at the IMP PAN throughout last thirty years. Personally, he specializes in several important sub–disciplines, like structural health monitoring techniques, vibration control, structural dynamics, composite structures, multifunctional materials, smart materials and structures, damage assessment of structures, working in these fields both theoretically and experimentally. In the past twelve years, his research was focused on the development and use of the Spectral Finite Element Method for damage assessment as well as smart materials applications. The aim of his research in guided wave propagation has been to develop a number of vibro–acoustic–ultrasonic methods for damage detection using smart sensor technologies. Those methods have demonstrated effectiveness and sensitivity to small cracks in metallic and composite structures, without restrictions on load, boundaries or temperature conditions.

Professor W. Ostachowicz published 310 archival international journal papers, 410 refereed international conference papers and over 200 technical reports, predominantly in the damage detection, structural health monitoring and advanced signal processing areas. Prof W. Ostachowicz published 6 monographs, 8 book chapters, 4 proceedings volume in the fields of structural dynamics and SHM. These have been published by worldwide famous publishers like Springer, Wiley, Kluwer, World Scientific, CRC Press, etc. The 310 papers currently represented on JCR Web of Science are uniformly distributed in the highest–quality international journals and have attracted 2980 citations (without self–citations). One of his paper published in the Journal of Sound and Vibration (Analysis of the effect of cracks on the natural frequencies of a cantilever beam, Vol. 150, 2, 191–201, 1991) has been cited 343 times.

RECENT PUBLICATIONS:

- ✓ Mieloszyk M., Majewska K., Ostachowicz W.: *Application of THz spectroscopy for localisation of fibre optics embedded into glass fibre reinforced composite*. COMPOSITE STRUCTURES, Vol. 209, pp. 548–560, published: FEB 1 **2019**

Abstract

Recently, in many industrial branches (e.g. aviation, marine or civil engineering) metal elements are replacing by composite ones. To ensure their reliability structural health monitoring systems also based on fibre optics sensors (embedded into or mounted on composite structure) are widely applied.

In the paper, THz spectroscopy technique was proposed for detection and localisation of glass fibre optics embedded into a glass fibre reinforced polymer. The analysis was performed on a four–layer sample manufactured by the infusion method. During this investigation, both the sample surfaces roughness as well as fibre optics arrangements (according to the THz spectrometer axes) were examined. For this purpose THz images of the internal structure of the sample were presented. Additionally, two methods (in time and frequency domains) for quick determining of fibre optics location are presented. The first one is based on local changes in signal amplitudes while the second – on differences in the power spectrum.

- ✓ Sikdar S., Fiborek P., Kudela P., Banerjee S., Ostachowicz W.: *Effects of debonding on Lamb wave propagation in a bonded composite structure under variable temperature conditions*. SMART MATERIALS AND STRUCTURES, Vol. 28 (1), published: JAN **2019**.

Abstract

Bonded composite structures are a special type of sandwich–like structures in which multiple carbon–fibre laminates are bonded with adhesives, and debonding can appear at the bond layer due to variable loading and uncertain operating conditions. This study aims to investigate the debonding effects on Lamb wave propagation in a bonded composite structure under variable ambient temperature conditions. In the process, a combined theoretical analysis, time–domain spectral element simulation and experimental analysis of elastic wave propagation in a carbon–fibre reinforced adhesively–bonded composite structure have been carried out. It is shown that theoretical analysis and spectral formulation are effectively able to capture the behaviour of Lamb modes in the healthy structure due to variations in ambient temperature. It is found that the primary anti–symmetric Lamb wave mode amplitude and velocity decrease with an increase in ambient temperature. Furthermore, the spectral formulation accurately captures the effects of debonding on the Lamb wave signals under variable temperature conditions that are consistent with the experimental results. Finally, temperature correction factors are proposed for the primary anti–symmetric mode velocity and amplitude difference calculations and the effectiveness of the factors is successfully verified for selected study cases.

- ✓ Malinowski P.H., Ostachowicz W.M., Touchard F., Boustie M., Chocinski–Arnault L., Gonzalez P.P., Berthe L., de Vasconcellos D.S., Sorrentino L.: *Study of plant fibre composites with damage induced by laser and mechanical impacts*. COMPOSITES PART B–ENGINEERING, Vol. 152, pp. 209–219, published: NOV 1 **2018**.

Abstract

Polymer composite materials provide good strength to weight ratio and tailored mechanical properties thanks to the reinforcing fibres. Until recently, the need for taking into account the whole life cycle of a composite structure was neglected and only the service aspects were important. Today, the designers of a new composite structure have to take into account the environmental aspects from the sustainability of raw materials to the management of end life products. There are recycling issues related to the most popular composites. A solution for the recycling issue can be sought in green composites with reinforcing fibre originating from plants. The behaviour of eco–composites, when

subjected to laser or mechanical impact loadings, is not well known yet. Short fibre composites were made with spruce fibres. Another set of samples was made of flax fibres. Also, a woven hemp fabric–based eco–composite was investigated. A fully synthetic woven composite was used for comparison with green composites. Mechanical impacts were performed by means of a falling dart impact testing machine. Laser impacts were made with a high power laser source. Four assessment techniques were employed in order to analyse and compare impact damage. Damage detection thresholds for each material and technique were obtained.

- ✓ Sikdar S., Ostachowicz W., Pal J.: *Damage–induced acoustic emission source identification in an advanced sandwich composite structure*. COMPOSITE STRUCTURES, Vol. 202, pp. 860–866, published: OCT 15 **2018**.

Abstract

This paper proposes an acoustic emission (AE) based real–time health monitoring framework to efficiently identify the probable damage initiation/propagation locations in advanced sandwich composite structures. Towards this, numerical simulations and laboratory experiments on damage–induced AE–wave propagation in an aramid honeycomb composite structure have been carried out using a randomly selected sensory network. The simulation results are successfully validated with laboratory experiments. Eventually, the damage–source/AE–source regions are efficiently identified by applying an evolutionary algorithm – Particle–Swarm–Optimization based monitoring framework, which uses the registered AE–signals from the sensory network. A thorough assessment of different AE–source locations was carried out to evaluate the performance and the robustness of the proposed online monitoring strategy. The results clearly represent the efficiency of the framework for localizing the AE–source locations in such advanced and complex structures. Moreover, the proposed framework is reliable, independent of sensor positions, and not dependent upon the operator's expertise.

- ✓ Soman R., Malinowski P., Majewska K., Mieloszyk M., Ostachowicz W.: *Kalman filter based neutral axis tracking in composites under varying temperature conditions*. MECHANICAL SYSTEMS AND SIGNAL PROCESSING, Vol. 110, pp. 485–498, published: SEP 15 **2018**.

Abstract

Structural Health Monitoring (SHM) systems allow early detection of damage which allows maintenance planning and reduces the maintenance cost. There is a lot of active research in the area for SHM of civil and mechanical structures. The SHM system should be low cost, suitable for continuous monitoring, able to detect small levels of damage, and insensitive to ambient loading, changes in ambient temperature, and measurement noise. Change in Neutral Axis (NA) has been used by several researchers as a damage sensitive feature. It has been shown to be sensitive to small levels of damage, and independent of the ambient loading. This paper aims at showing the insensitivity of the NA to ambient condition changes.

This paper demonstrates a methodology for overcoming the effect of temperature on the accurate tracking of the NA. A multi –rate Kalman Filter (KF) has been used for data fusion from temperature and strain sensors. The paper shows that through the use of KF one can easily compensate the effect of temperature on the observability of the NA. The work applies the methodology on a finite element (FE) model of a glass fiber–epoxy composite as well as validation through actual experiments. Based on the results obtained, it is apparent that the NA tracking using KF allows stable estimation even in changing

temperature conditions and as such shows that NA location can indeed be used as a damage sensitive feature.

- ✓ Kudela P., Ostachowicz W.: *Comparison of Lamb wave focusing performance using wave dispersion–compensated actuation and piano–concave lenses*. JOURNAL OF APPLIED PHYSICS, Vol. 124 (9), published: SEP 7 **2018**.

Abstract

Lamb waves are often used for damage detection in structures. Hot–spot monitoring via wave focusing is considered in this study, which can be achieved by using a piano–concave aspherical lens. Once attached to the plate, the lens modifies the effective plate thickness, and therefore changes the Lamb wave characteristics, such as wavenumber and phase velocity, providing a convenient way of controlling Lamb waves. Another possibility for focusing Lamb waves is to use multiple actuators and design dispersion pre–compensated excitation signals with an embedded time delay. These two approaches can be combined together. We conducted numerical simulations using the time–domain spectral element method based on the 3D elasticity theory and demonstrated that the A0 mode of Lamb waves could be focused on the desired focal point. We compared the efficacies of the piano–concave lens approach, the dispersion pre–compensated focusing approach, and a combination of both approaches, emphasizing the advantages and disadvantages of each method.

- ✓ Soman R., Mieloszyk M., Ostachowicz W.: *A two–step damage assessment method based on frequency spectrum change in a scaled wind turbine tripod with strain rosettes*. MARINE STRUCTURES, Vol. 61, pp. 419–433, published: SEP **2018**.

Abstract

The paper presents a proof of concept of a two–step methodology for the damage detection and localization in a scaled model of an offshore support structure. Two damage scenarios have been simulated for validating the methodology. The first damage scenario investigated is deterioration of the support condition which is simulated by removing the attachment of a leg of a tripod to the table and the second scenario is simulated by unbolting the flange to create an artificial circumferential crack in the upper brace of the tripod structure.

The strain measurements have been obtained from a network of Fibre Bragg Grating (FBG) sensors bonded to the model. The damage detection is carried out in the first step using the root mean square deviation (RMSD) estimator. If the RMSD value is above a certain threshold, damage is said to be detected. Experimental results show that additional peaks appear in some frequency regions revealing vibration modes which are associated with damage in the structure. Applying the RMSD estimator to the regions where new peak has emerged it is possible to detect the damage. Once the damage is detected the damage isolation factor (DIF) is used for the damage isolation (level II damage detection). The DIF is based on the RMSD as well, and involves normalization using the rosette set values. Based on the results, it is seen that the DIF shows good localization performance. This good performance can be attributed to the ability of the parameter to overcome biases due to higher relative amplitude of vibration of some rosettes.

- ✓ Kudela P., Radzienski M., Ostachowicz W.: Yang Z.B.: *Structural Health Monitoring system based on a concept of Lamb wave focusing by the piezoelectric array*. MECHANICAL SYSTEMS AND SIGNAL PROCESSING, Vol. 108, pp. 21–32, published: AUG **2018**.

Abstract

Piezoelectric transducer arrays are utilized in Structural Health Monitoring systems as a means for excitation and sensing of elastic waves. Anomalies of propagating waves have enabled to develop damage detection algorithms. Depending on actuation–sensing strategies these algorithms can be classified as pitch–catch and pulse–echo. Despite many signal processing methods such as delay–sum, time–reversal, probability–based diagnostic imaging, etc. the spatial damage information provided by the actuator–sensor paths to reconstruct the damage image is limited. A novel strategy based on Lamb wave focusing is proposed in order to increase damage imaging resolution. In the proposed method all actuators are used at the same time exciting specially designed waveforms so that inspect one specific point of the structure. Damage map is created by applying appropriate signal processing. It uses dispersion curve of selected Lamb wave mode for dispersion compensation. The dispersion curve is acquired by using laser scanning Doppler vibrometer. The damage indicator is calculated based on the energy of compensated signals registered by sensors. It is shown that apart from high energy level at excitation point, energy is concentrated exactly in the damaged region. An example of crack detection and visualization in an aluminum plate is shown confirming the accuracy of the proposed method. Also the proposed method is compared to well–established delay–and–sum algorithm.

- ✓ Mieloszyk M., Majewska K., Ostachowicz W.: *Localisation of embedded water drop in glass composite using THz spectroscopy*. SMART STRUCTURES AND SYSTEMS, Vol. 21(6), pp. 751-759, published: JUN **2018**.

Abstract

Glass fibre reinforced polymers (GFRP) are widely exploited in many industrial branches. Due to this Structural Health Monitoring systems containing embedded fibre optics sensors are applied. One of the problems that can influence on composite element durability is water contamination that can be introduced into material structure during manufacturing. Such inclusion can be a damage origin significantly decreasing mechanical properties of an element. A non-destructive method that can be applied for inspection of an internal structure of elements is THz spectroscopy. It can be used for identifications of material discontinuities that results in changes of absorption, refractive index or scattering of propagating THz waves. The limitations of THz propagation through water makes this technique a promising solution for detection of a water inclusion. The paper presents an application of THz spectroscopy for detection and localisation of a water drop inclusion embedded in a GFRP material between two fibre optics with fibre Bragg grating sensors. The proposed filtering method allowed to determine a 3D shape of the water drop.

Biological Cell Walls with Atomic Force Microscopy and Scanning Acoustic Microscopy

by Bernhard R. Tittmann, Member EUAS

Short Biography

Schell Professor of Engineering, Emeritus
Director of Engineering Nanostructure Characterization Center
The Pennsylvania State University

Academic Training

B.S. (Physics and Mathematics), George Washington University, Washington, DC, 1957
Ph.D. (Solid State Physics), University of California at Los Angeles, CA, 1965

***Teaching Experience**:*

Professor, The Pennsylvania State University, University Park, PA 16802, 1989-present;
Visiting Professor, Fall 2017, University of California, Santa Barbara, CA
Visiting Professor, Spring 1995-1997. Johannes Kepler University, Linz, Austria.
Visiting Professor, University of Paris III, Physics Department, 1977, 1979, 1982.
Assistant Professor (in residence), 1965-1966. Physics Department, University of California at Los Angeles, CA.

Industrial Experience

Manager, Materials Characterization. Science Center, Rockwell Intern., 1979 - 1989.
Member Staff, Materials Mechanics Group. Science Center, Rockwell, 1966-1977.
Howard Hughes Fellow – Microwave Antenna Dept.; Hughes Research Lab., Culver City, CA, 1957-1962.

Professional Societies and Activities

American Ceramic Society (ACS), Member 1995 – present
American Society for Metals (ASM) International, Member 1993, Fellow 2006 – present
American Society of Nondestructive Testing (ASNT), Member 1980 – present
Materials Research Society (MRS), Member, 1995 – present
American Society of Mechanical Engineers (ASME), Member, 2001 – present
Acoustical Society of America (ASA), Fellow, 2001 – present
Technical Program Committee - Standing Member, 1999 to present
Institute of Electrical and Electronics Engineering (IEEE), Fellow, 1990 – present
Distinguished IEEE – UFFC Lecturer, June 1998 – December 1999
Vice-Chair of Awards Committee, IEEE – UFFC, 2003-present
International Society for Optical Engineering (SPIE), Senior Member

Awards/Honors

Marquis Who's Who Albert Nelson Marquis Lifetime Achievement Award 2018
Top 100 Registry Professors of the Year, 2018
EU Academy of Sciences, January 2018
Schell Professor, Emeritus July, 2017.
Endowed Chair at Penn State College of Engineering Schell Professor of Engineering 1989 (renewed 5 times) to June, 2017.
IEEE-UFFC Distinguished Service Award 2017
IEEE-UFFC Invited Speaker at 2017 Int. Ultrasonics Symposium, Washington, D.C.
Named Consulting Editor of Archives of Acoustics, Polish Academy of Sciences, Warsaw, 2003
Penn State Engineering Society Outstanding Research Award, 1998
Senior Fulbright Fellowship, Spring and Summer 1999
Rockwell Award for Highest IR&D Score Rockwell Science Center (1988)

NASA Principal Investigator Award for "Elastic and Anelastic Properties of Lunar Rock (1979)."
Howard Hughes Fellow (1957-1962).
Phi Beta Kappa (1957).
Graduation Cum Laude (1957).
G. Washington Tuition Scholarship (1953-1957).
Accomplishment
Graduated 11 PhD students and 25 MS students.
Citations 4028; h-index 32
Nearly 500 publications including refereed journal publications and refereed Proceedings.
8 Patents

1. Summary

In this research our group has the goal to demonstrate the feasibility of our Atomic Force Microscope (AFM) and our High Frequency Scanning Acoustic Microscopy (HF-SAM) as tools to characterize biological tissues. Both the AFM and the HF-SAM have shown to provide imaging (with different resolution) and quantitative elasticity measuring abilities. Plant cell walls with minimal disturbance and under conditions of their native state have been examined with these two kinds of microscopy. The sample preparation is focused here on epidermal peels of onion scales and celery epidermis cells which were sectioned for the AFM to visualize the inner surface (closest to the plasma membrane) of the outer epidermal wall. The nanometer-wide cellulose microfibrils orientation and multilayer structure were clearly observed. The microfibril orientation and alignment tend to be more organized in older scales compared with younger scales. The onion epidermis cell wall was also used as a test analogue to study cell wall elasticity by the AFM nanoindentation and the HF-SAM *V(z)* feature. The novelty in this work was to demonstrate the capability of these two techniques to analyse isolated, single layered plant cell walls in their natural state. AFM nanoindentation was also used to probe the effects of EDTA (Ethylenediaminetetraacetic acid), and calcium ion treatment to modify pectins in cell walls. The results suggest a significant modulus increase in the calcium ion treatment and a slight decrease in EDTA treatment. To complement the AFM measurements, the HF-SAM was used to obtain the *V(z)* signatures of the onion epidermis. These measurements were focused on documenting the effect of pectinase enzyme treatment. The results indicate a significant change in the *V(z)* signature curves with time into the enzyme treatment. Thus, AFM and HF-SAM open the door to a systematic non-destructive structure and mechanical property study of complex biological cell walls. A unique feature of this approach is that both microscopes allow the biological samples to be examined in their natural fluid (water) environment. This report gives an abbreviated description into our research.

2. Introduction

Plant cell walls serve a variety of important biological functions for plants, such as providing mechanical support and determining their size and shape. They have also been an interesting subject for engineering applications. Plant cell walls are essential in various commercial products such as paper, textile, plastic, etc. Most recently, they have gained intensive attention as potential sources for biofuel. Also, the sophisticated composite structure, naturally occurring in cell walls, inspires innovative designs of engineering materials. All these applications require understanding of the composite structure of cell walls and their mechanical properties. Primary cell walls are formed during the growth and division of plant cells. They provide mechanical support for the cells and can expand to allow cells to grow. Primary plant cell walls are polysaccharide-rich complex structures. The wall contains three main components: cellulose, hemicelluloses and pectin. Cellulose microfibrils are embedded in a highly hydrated polysaccharide matrix which consists of hemicelluloses and pectin. Cellulose is comprised of many parallel chains of 1,4-glucan, which make cellulose crystalline, strong and indigestible. Cellulose microfibrils serve as reinforcement material of cell wall composite. Cellulose microfibrils are several nano-meter in thickness and have varied length. Hemicellulose is also a polysaccharide, but it is typically made up of chains of xylose interspersed with side chains containing arabinose, galactose, mannose, glucose, acetyl, and other

sugar groups, depending on the plant type. Hemicelluloses separate microfibrils from each other but may tether them together into a cohesive network. Pectin is a gel phase that embeds the cellulose-hemicelluloses network.

3. AFM Imaging of hydrated cell walls

Figure 1 shows the typical AFM topography images of onion epidermis wall and celery (Apium graveolens L.) parenchyma cell walls. In the topography images, the nm-wide cellulose microfibrils orientation and multilayer structure were clearly observed. In our work of imaging epidermis cell wall of different onion scales, the AFM images showed that cellulose microfibrils exposed at the innermost surface of the abaxial epidermis are oriented perpendicular to the bulb axis in the outer scales and more dispersed in the inner scales of onion bulb.

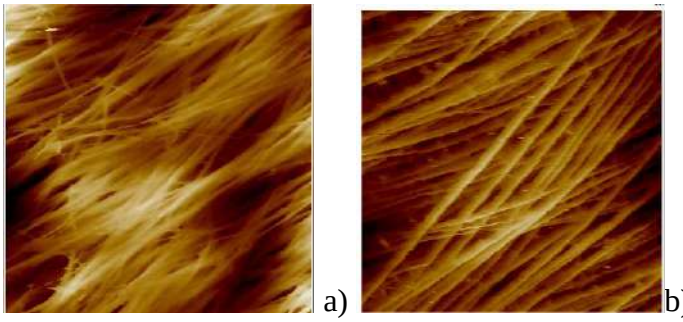

Fig.1 AFM images of the abaxial epidermal cell wall of a) the onion scale and b) celery epidermis walls. a) 1μm square and b) 500 nm square of the wall surface clearly show cellulose microfibril and matrix detail.

Plant cell walls are complex composites which require delicate instruments and special techniques to study their structures and properties. The analysis of micro- or nano- mechanical properties of plant cell walls has become increasingly important in understanding cell wall structure and cell growth. Because of its micro-scale tip size, indentation technique can investigate the mechanical properties of thin, small and heterogeneous materials. Nanoindentation has been a new application tool on cellulose fibers and plant cell walls. hardness and Young's modulus of spruce cell-wall, bamboo cell walls, individual wood fibers and crop stalks cell walls were examined. These experiments were done with add-on force transducers or special indenter testing systems. However, in traditional nanoindentation experiments, samples were dehydrated and many were embedded in epoxy resin. Such sample preparations may cause undesired modifications and influence the mechanical properties of the cell walls. No conclusive results were reached on the cell mechanical properties with the effect of turgor pressure. The aim of our research is to focus on the elastic properties of cells walls isolated from onion scales using AFM based nanoindentation and scanning acoustic microscopy to assess the feasibility of these methods for further study of plant cell walls. Here the focus is further on the freshly peeled single-layer onion abaxial epidermis wall tested in liquid mode. The samples are independent of the turgor pressure influence and reflect only the properties of hydrated cell wall in its natural condition.

With its pico-newton force sensitivity and nanometer displacement accuracy, the AFM has been recognized as a promising tool to for studying materials properties. AFM with force-distance curve measurement for nanoindentation has emerged as a useful tool measuring the elastic moduli of biological samples. An AFM force-distance (F-D) curve is a plot of tip-to-sample forces versus the extension of the piezoelectric scanner measured with a position-sensitive photo detector. The F-D curve provides information of important mechanical properties such as adhesion, contaminants, viscosity, and local variations in the elastic properties of the surface.

The Hertz model is used as the theoretical model for f-d curve analysis. The Hertz model assumes that the sample is isotropic, elastic and occupies infinite half space. The elastic modulus E can be obtained by a fit to the experimental F-D curve using the Hertz model. The F-D curve obtained by AFM nanoindentation is in fact a force- piezo displacement curve. Knowing that $x=$

F/k, where *k* is the cantilever spring constant, we can easily obtain relationship between recorded force F and recorded piezo displacement *D*:

$$F = \frac{E}{1-\nu^2}\frac{\tan\alpha}{\sqrt{2}}(D - \frac{F}{k})^2 \quad (3)$$

By fitting the experimental F-D retrace curves, we can get the sample's elastic modulus *E*. Figure 2 shows a sample F-D curve fitting result. The experimental F-D retrace curve and fitted curve from the Hertz model are in good agreement.

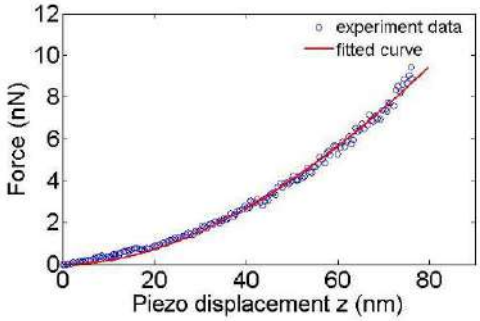

Fig. 2 A sample of F-D curve fitting. Experiment data in blue dots and fitted data in the red curve from the Hertz model showed good agreement.

4. Imaging with frequency scanning acoustic microscopy HF-SAM.

In contrast to Scanning Electron Microscopy (SEM), Optical or Scanning Laser Confocal Microscopy (SLCM), high frequency scanning acoustic microscopy (HF SAM) is capable of imaging not only the surface but also the shallow subsurface regions of materials with high resolution. For example, at 500 MHz the resolution in water at Standard Temperature and Pressure is about 1.5 um. For the focus below the surface of a biological specimen the resolution is approximately 2 micron depending on the acoustical properties of the specimen. Imaging bonds between dissimilar polymers is a challenging task since the image contrast must be based on at least two mechanisms: (1) the contrast resulting from the dissimilar acoustic impedances of the different polymers and (2) the contrast due to absorption of acoustic waves in the material. Conventional acoustic microscopy typically operates in the 20 MHz to 200 MHz range with the use of focused transducers operating in the pulse wave mode. By contrast, HF SAM operates in the 0.4 GHz to 2 GHz range in the long tone burst mode which allows correspondingly much higher resolution. More importantly, the high numerical aperture lens when brought close to the surface produces leaky surface acoustic waves which are sensitive to the presence of changes in structure and materials and mark them in high intensity contrast.

The HF SAM uses a mechanically scanning, acoustic lens system operating in a pulse-echo reflection mode. Fig. 3 are displayed typical HF SAM images of onion epidermal walls at a frequency of *f*= 600 MHz and at two different scales. The white lines in (a) are identified as cuticle structures located between adjacent cell walls making up the risers in the "shoe-box-like" structure.

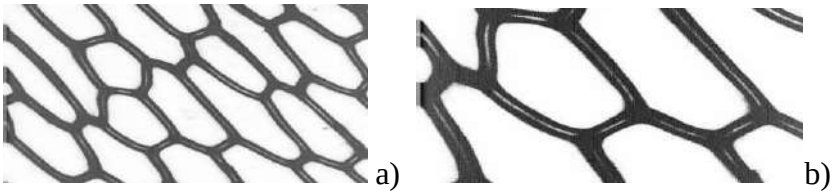

Fig. 3 Typical acoustic images of onion epidermal walls at a frequency of 600 MHz. The white lines are identified as cuticle structures located between adjacent cell walls making up the risers in the "shoe-box" structure. In (a) the scan width is 1 mm, whereas in (b) the scan width is 0.5 mm.

In addition to contrast variations provided by elastic properties of materials, another important usage of high frequency HF SAM is measuring the velocity of surface acoustic waves. Following well-known procedures to obtain, measure, and interpret *V(z)* curves, the longitudinal wave velocities were obtained by implementing a computer parameter-fitting technique. The algorithm of the *V(z)* curve simulation is described in the following steps. First, initialize parameters of acoustic lens, specimen (thinly sectioned biological tissue), and soda-lime substrate. Second, calculate parameters of acoustic field at the back focal plane, pupil function of the lens, and reflectance function. Third, calculate and draw the *V(z)* curve. The velocity of the longitudinal wave velocity of water was set as 1,487 m/s. Based on the previous research study, the speed of sound in most plant cells is quite constant and close to that of water, with ultrasound velocities are in the range of about 1600 m/s. Therefore, the longitudinal velocity of the tissue (thickness: 8μm) was set to a range from 1540 m/s to 1650 m/s. Moreover, the plant cell wall density is set within a range of 1.3 – 1.6 (10^3 kg m^{-3})**.** A Soda-lime glass slide was chosen as the substrate, its velocities of longitudinal and shear waves are 6,000 m/s and 3200 m/s respectively.

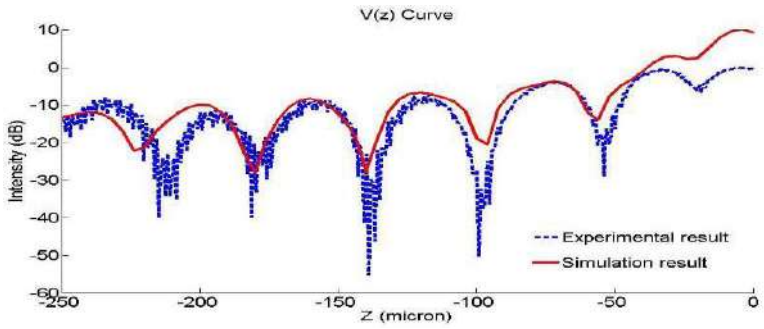

Fig.4 A typical experimental V(z) curve shown in blue line and the simulated V(z) curve in red line. The curve was obtained at room temperature on hydrated onion epidermis. The vertical axis is the intensity of the received signal. The horizontal axis is the defocusing distance of the lens. z=0 represents the position of the lens when it is focused on the top surface of the specimen. The curves are obtained as the lens is moved deeper into the interior of the specimen. Further analysis gives the effective elastic modulus.

5. Conclusions

In summary, this is a description of of our research with two methods in advanced microscopy. The two methods stand out from other microscopies in that they are used with water-immersed samples. The two methods are acoustic microscopy for microscale resolution and atomic force microscopy for nanmeter resolution. The two methods are not restricted to but are demonstrated for biological samples, in particular plant cell walls, which are currently of particular interest. The interest arises in the desire to understand the composition and properties of plant cell walls which are the fundamental building blocks for all natural plants ubiquitous around the globe and are therefore of great importance to mankind and civilization.

Drills: Science and Technology of Advanced Operations

by Viktor P. Astakhov, Member EUAS

Short Biography
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Tool Research and Application Manager – Research Professor
General Motors Propulsion Division Business Unit of PSMI Okemos, MI, USA
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Viktor P. Astakhov earned his PhD in mechanical engineering from Tula State Polytechnic University, Tula-Moscow, USSR-Russia, in 1983. He was awarded a DSci designation (Dr. habil., Docteur d'État) in 1991 and the title "State Professor of Ukraine" in 1991 for the outstanding service rendered during his teaching career and for the profound impact his work had on science and technology. An internationally recognized educator, researcher, and mechanical engineer, he has won a number of national and international awards for his teaching and research. In 2011, he was elected to the SME College of Fellows.
Dr. Astakhov currently serves the tool research and application manager research professor of the General Motors Business Unit of PSMI and Professor, St. Petersburg State Polytechnic University, St. Petersburg, Russia. As a professor, he has been involved in supervising graduate students at Michigan State University. He has published monographs and textbooks, book chapters, and many papers in professional journals as well as in trade periodicals. He has authored the following books: Geometry of Single-Point Turning Tools and Drills: Fundamentals and Practical Applications, Tribology of Metal Cutting, Physics of Strength and Fracture Control, and Mechanics of Metal Cutting. He serves as associate editor of International Journal of Manufacturing, Materials and Mechanical Engineering (IJMMM) and International Journal of Machining and Machinability of Materials (IJMMM), board member, reviewer, and advisor for more than 20 international journals and professional societies.

Selected publications:

Astakhov V.P., Drills: Science and Technology of Advanced Operations, CRC Press, 2014

In a presentation that balances theory and practice, Drills: Science and Technology of Advanced Operations details the basic concepts, terminology, and essentials of drilling. The book addresses important issues in drilling operations, and provides help with the design of such operations. It debunks many old notions and beliefs while introducing scientifically and technically sound concepts with detailed explanations.

The book presents a nine-step drilling tool failure analysis methodology that includes part autopsy and tool reconstruction procedure. A special feature of the book is the presentation of

special mechanisms of carbide (e.g. cobalt leaching) and polycrystalline (PCD) tool wear and failure presented and correlated with the tool design, manufacturing, and implementation practice. The author also introduces the system approach to the design of the drilling system formulating the coherency law. Using this law as the guideline, he shows how to formulate the requirement to the components of such a system, pointing out that the drilling tool is the key component to be improved.

Teaching how to achieve this improvement, the book provides the comprehensive scientific and engineering foundations for drilling tool design, manufacturing, and applications of high-performance tools. It includes detailed explanations of the design features, tool manufacturing and implementation practices, metrology of drilling and drilling tools, and the tool failure analysis. It gives you the information needed for proper manufacturing and selection of a tool material for any given application.

Astakhov V.P., Joksch, S., Metal Working Fluids: Fundamentals and Recent Advances,, Woodhead Publishing Limited, Cambridge, UK, 2012

Metal working fluids (MWFs) provide important functions such as lubrication and cooling in the machining of metals. This book reviews the issues surrounding the use of fluids for cutting and grinding throughout the metal working process, from selection and testing to disposal.

The book opens with chapters considering the mechanism and action, selection and delivery of MWFs to the machining zone before moving onto discuss the many issues surrounding MWFs during machining such as selection of the proper MWF, environmental concerns, supply methods, circulation and monitoring. The final chapters discuss the maintenance, replacement and disposal of MWFs.

Metalworking fluids (MWFs) for cutting and grinding is an invaluable reference tool for engineers and organizations using metal cutting/machining in the manufacturing process as well as machine designers/manufacturers and machining fluid/chemical suppliers. Chapters consider the mechanism and action, selection and delivery of MWFs to the machining zone Environmental concerns, supply methods, circulation and monitoring are also discussed Written by distinguished editors and international team of expert contributors

Astakhov, V.P., Geometry of Single-Point Turning Tools and Drills: Fundamentals and Practical Applications. (Springer, 2010).

Tools for metal cutting have many shapes and features, each of which is described by its angles or geometries. The selection of the right cutting tool geometry is critical because it directly affects the integrity of the machined surface, tool life, power needed for machining, and thus the overall machining efficiency. Geometry of Single-Point Turning Tools and Drills outlines clear objectives of cutting tool geometry selection and optimization, using multiple examples to provide a thorough explanation.

The establishment of clear bridges between cutting theory, tool geometry, and shop practice, reveals individual and combined influences of the parameters of cutting tool geometry on cutting tool performance and on the outcomes of a machining operation. The three basic systems of considerations of tool geometry – namely, tool-in-hand, tool-in-machine (holder) and tool-in-use – are covered, and the transformations between these systems are established.

Geometry of Single-Point Turning Tools and Drills addresses several urgent problems that many present-day tool manufacturers, tool application specialists, and tool users, are facing. It is both a practical guide, offering useful, practical suggestions for the solution of common problems, and a useful reference on the most important aspects of cutting tool design, application, and troubleshooting practices.

Covering emerging trends in cutting tool design, cutting tool geometry, machining regimes, and optimization of machining operations, Geometry of Single-Point Turning Tools and Drills is an

indispensable source of information for tool designers, manufacturing engineers, research workers, and students

Astakhov, V.P., Tribology of Metal Cutting, Elsevier: London, 2006.

Tribology of Metal Cutting deals with the emerging field of studies known as Metal Cutting Tribology. Tribology is defined as the science and technology of interactive surfaces moving relative each other. It concentrates on contact physics and mechanics of moving interfaces that generally involve energy dissipation. This book summarizes the available information on metal cutting tribology with a critical review of work done in the past.

The book covers the complete system of metal cutting testing. In particular, it presents, explains and exemplifies a breakthrough concept of the physical resource of the cutting tool. It also describes the cutting system physical efficiency and its practical assessment via analysis of the energy partition in the cutting system. Specialists in the field of metal cutting will find information on how to apply the major principles of metal cutting tribology, or, in other words, how to make the metal cutting tribology to be useful at various levels of applications. The book discusses other novel concepts and principles in the tribology of metal cutting such as the energy partition in the cutting system; versatile metrics of cutting tool wear; optimal cutting temperature and its use in the optimization of the cutting process; the physical concept of cutting tool resource; and embrittlement action.

Komarovsky, A.A. and Astakhov, V.P., Physics of Strength and Fracture Control: Fundamentals of the Adaptation of Engineering Materials and Structures to Operating Conditions, CRCPress, 2002

Still passive and for the most part uncontrollable, current systems intended to ensure the reliability and durability of engineering structures are still in their developmental infancy. They cannot make corrections or recondition materials, and most material and structural failures cannot be predicted. Accidents-and catastrophes-result.

Physics of Strength and Fracture Control: Adaptation of Engineering Materials and Structures introduces a new physical concept in the science of the resistance of materials to external effects, a concept that opens completely new avenues for improving the strength and safety of engineered objects. Based on a thermodynamic equation of state of solids derived by the author, the approach provides a general methodology for treating all the physical and mechanical properties of materials, regardless of their nature and physical state. The author shows that this approach enables the control of the stressed-deformed state both to prevent failures and fractures and to promote them for easier shaping of materials. He uses this methodology to present and discuss non-traditional but practical ways of solving real-world problems.

Of enormous theoretical and practical significance, this groundbreaking work ushers in a new stage in the science of material strength. It opens the door to systematic ways to design materials, control their operating properties, and predict their behavior under specific operating conditions.

Astakhov V.P., Metal Cutting Mechanics, CRC Press, 1998/1999.

Metal Cutting Mechanics outlines the fundamentals of metal cutting analysis, reducing the extent of empirical approaches to the problems as well as bridging the gap between design and manufacture. The author distinguishes his work from other works through these aspects: considering the system engineering of the cutting process identifying the singularity of the cutting process among other closely related manufacturing processes by chip formation, caused by bending and shear stresses in the deformation zone suggesting a distinctive way toward predictability of the metal cutting process devoting special attention to experimental methodologyMetal Cutting Mechanics provides an exceptional balance between general reading and research analysis,

presenting industrial and academic requirements in terms of basic scientific factors as well as application potential.

Astakhov V.P., Patel S. (2018). 1. Efficient drilling of high-silicon aluminum alloys. In J. Paulo Davim (Editor), Drilling Technology: Fundamentals and Recent Advances (pp. 1–36). Berlin, Boston: De Gruyter.

This chapter presents the most important features of high-penetration rate (HPR) drilling of high-silicon aluminum alloys (HSAA). It explains a necessity of implementation of HPR tools and well-designed machining operations that has become possible due to development of a number of new tool materials and coatings, new cutting inserts and tool designs, new tool holders, powerful precision machines, part fixtures, advanced controllers and so on. As the penetration rate is the product of the tool's (workpiece) rotational speed and cutting feed, the major constraints of these two parameters are considered and a number of practical recommendation for increasing the penetration rate are made as the first level of the analysis. At the second level of the analysis, the correlations between the chemical composition and physical properties of HSAA and drilling tool/process parameters are explained. As HSAA are die casting alloys, the casting defect and their influence on tool performance are analyzed. It is pointed out that polycrystalline diamond (PCD) is a material of choice for HPR drilling tools for HSAA. The common problems with the existing PCD drilling tool are analyzed and the basic design of a cross-PCD drill is suggested.

Astakhov V.P. (2018) Mechanical Properties of Engineering Materials: Relevance in Design and Manufacturing. In: Davim J. (eds) Introduction to Mechanical Engineering. Materials Forming, Machining and Tribology. Springer, Cham

The chapter provides an introduction to mechanical engineering, covering fundamental concepts of mechanical properties of materials and their use in the design and manufacturing. It first explains the notion of mechanical properties of materials and then elaborates on the proper definition of most relevant properties as well as materials testing to obtain these properties. The role of mechanical properties at the design stage in form of the design criterion is explained. The use of material properties to assess equivalent stress and strain in complex loading conditions is revealed. At the manufacturing stage, the notion of additive (material is added to the workpiece), neutral (the volume of the workpiece is preserved), and substantive (the volume of the workpiece is reduced) processes is introduced. The relevant properties of materials in the neutral (forming) and substantive (cutting) processes are considered.

Astakhov V.P., Improving sustainability of machining operation as a system endeavor, In book: Sustainable Machining, Edited by J.P. Davim, Springer 2017, pp. 1-29.

This chapter elaborates on the attractiveness of the notion of sustainability in machining and points out needs for its improvement. It explains that the chief areas of further improvement in sustainability of machining operations are improvement in modeling of the cutting process and thus in the design of practical machining operations; system considerations of measures to enhance sustainability of machining; and development of proper metrics for sustainability assessment. As such, the proper modeling of machining operation plays the most important role as it allows realizing the idea of virtual machining as a keystone of machining sustainability. The chapter argues that one of the most common mistakes made in known an attempt to improve sustainability of machining operations is a nonsystem approach to the analysis of the result. The latter was exemplified by considerations of errors made in implementation practices of dry and near-dry machining as well in the reduction of the volume of the work material being removed by machining, i.e., the use of near-net-shape blanks.

Astakhov V.P., Xiao X. The principle of minimum strain energy to fracture of the work material and its application in modern cutting technologies, In book: Metal Cutting Technology, Edited by J.P. Davim, De Gruyter Publishers 2016, pp. 1-35.

This chapter presents introduces, explains, and exemplifies an entirely new physics-based 'flagship' concept, called the Principle of Minimum Strain Energy at Fracture (PMSEF) to be used in metal cutting research, design of practical machining operations and cutting tools, as well as assessment composition and properties of work materials in terms of their machinability. The concept is based on the definition of metal cutting as purposeful fracture of the work material, and on the fact that the energy of plastic deformation of the layer being removed in its transformation into the chip constitutes up to 75% of the total energy supplied to the cutting system. According to PMSEF, the energy of plastic deformation can be reduced by altering stress triaxiality in the deformation zone. The application of PMSEF leads to greater tool life, lower temperatures in the machining zone and cutting force, higher accuracy of machining. The following tasks are proposed: (1) develop a physics based work material constitutive model with parameters determined at conditions that pertinent to metal cutting process; (2) validate the constitutive model in metal cutting simulations against experimental results; (3) use the developed models to investigate typical machining operations to understand their underline mechanisms; and (4) validate the hypothesis of using the PMSEF as an optimization criterion for the design of cutting tools and process for improving machinability; (5) Develop and validate a physics based model of contact conditions at the tool-chip and tool workpiece interfaces. Using this model, verify the concept of physical resource of the cutting tool as a consequence of PMSEF; (6) To facilitate and simplify practical implementation of PMSEF, formulate, derive, and verify the basic similarity number in metal cutting to be used in machining practice to improve process predictability and efficiency; (6) Formulate guidelines for the development/design of high-performance cutting tools and process for improving machinability using MSEF as the goal under real-life constrains (acceptable part quality, tool life, required machining productivity and so on).

Astakhov V.P., Submicro and nanostructuring of materials by severe plastic deformation, Chapter 1 in book: Modern Manufacturing Engineering, Edited by J.P. Davim, Springer 2015, pp. 1-40.

This chapter discusses the development of the metallurgical structure of submicro and nanostructured metallic materials in Severe Plastic Deformation (SPD). Particular attention is paid to Equal-Channel Angular Pressing (ECAP) as the most feasible way to achieve the major objectives of grain refinement, distinguished as strength enhancement, superplasticity, and improvement in creep resistance. The need and essence of the multi-pass process is explained in detail. Particular attention is paid to the deformation mode in SPD. It is shown that the discussed objectives can be achieved if this deformation mode is simple shear. The chapter also presents the development and modeling of large strain extrusion machining (LSEM), comparing the results obtained in this process with those in ECAP

Sensing with Quantum Cascade Laser and Detector Systems

by Erich Gornik, Member EUAS

Short Biography

Erich Gornik *received his Ph.D. degree in Physics in 1972. He was a Postdoctoral Fellow at Bell Laboratories, Holmdel, USA, from 1975 to1977. In 1979, he has been appointed Professor for Experimental Physics at the University of Innsbruck. In 1988, he became Professor for Semiconductor Physics and Director at the Walter Schottky Institute of the Technical University Munich. From 1993 until 2012, he was Full Professor for Semiconductor Electronics and Director of the Micro-and Nanostructure Center (ZMNS) at the Technical University of Vienna and since then he is emeritus Professor. From 2003 to 2008 he was managing director of the Austrian Research Centers.*

He has spent several Research Professorships at numerous international research institutions and has received various awards; among others, he is Fellow of the American Physical Society since 1995. In 1997 he received the "Wittgenstein Award" of the Austrian Government and in 2000 the "Erwin Schrödinger Award" of the Austrian Academy of Science. He has supervised more than 150 Master and PhD students. Further achievements are 523 refereed publications, 236 conference proceedings, 90 invited and plenary lectures at international conferences, 7 Patents, h-factor 46.

Sensing with Quantum Cascade Laser and Detector Systems

Erich Gornik

Presentation at the Osaka Institute of Technology, July 26.2018 and Osaka University, July 30. 2018

Optical sensors for mid-infrared spectroscopy are widely used in industrial and environmental monitoring as well as medical and biochemical diagnostics. A sensor concept, based on a bi-functional quantum cascade heterostructure, for which the differentiation between laser and detector is eliminated, enables mutual commutation of laser and detector, simplifies remote sensing setups and facilitates a crucial miniaturization of sensing devices.

Liquid sensing utilizing bi-functional quantum cascade lasers/detectors (QCLDs) can be realized on a single chip. A QCL active region design with an additional detection capability at the laser emission wavelength allows a straightforward integration, where different parts of the chip are used for lasers and others for detectors. The performance of such bi-functional designs has been optimized to reach a similar laser performance as conventional QCLs, allowing for high duty cycle operation at room temperature.

Typical analyte interaction lengths for gas sensing are in the range of tens of centimeters or more and exceed the common semiconductor chip sizes. Our gas sensing approach incorporates surface-active lasers and detectors. The latest demonstrator consists of two concentric ring QCLDs with second order distributed feedback (DFB) gratings on top of the waveguides. These DFB gratings facilitate vertical light emission and detection in the biased lasing and unbiased detector configuration, respectively. The two rings emit at two different wavelengths, which provides room temperature lasing and detection of two wavelengths monolithically integrated on the same chip.

Monolithically integrated quantum cascade laser and detection devices

Gottfried Strasser and Erich Gornik

Conference: Advances in mid-IR based sensing: sources, detectors and applications

Vienna, Austria, 4.-6. April 2018

Optical sensors for mid-infrared spectroscopy are widely used in industrial and environmental monitoring as well as medical and biochemical diagnostics. Conventional optical sensing setups include a light source, a light-analyte interaction region and a separate detector. We present a sensor concept, based on a bi-functional quantum cascade heterostructure, for which the differentiation between laser and detector is eliminated. This enables mutual commutation of laser and detector, simplifies remote sensing setups and facilitates a crucial miniaturization of sensing devices.

Liquid sensing utilizing bi-functional quantum cascade lasers/detectors (QCLDs) can be realized on a single chip [1]. A QCL active region design with an additional detection capability at the laser emission wavelength allows a straightforward integration, where different parts of the chip are used for lasers and others for detectors. The performance of such bi-functional designs has been optimized to reach a similar laser performance as conventional QCLs, allowing for high duty cycle operation at room-temperature.
Sensing liquids utilizes surface plasmon polaritons to allow a strong interaction within a short distance. Different distributed-feedback-laser/waveguide/detector units can be combined on a single chip, to use the inherent selectivity of the mid-infrared region.

Typical analyte interaction lengths for gas sensing are in the range of tens of centimeters or more and exceed the common semiconductor chip sizes. Our gas sensing approach incorporates surface-active lasers and detectors [2]. The latest demonstrator consists of two concentric ring QCLDs with second order distributed feedback (DFB) gratings on top of the waveguides. These DFB gratings facilitate vertical light emission [3] and detection in the biased lasing and unbiased detector configuration, respectively. The two rings emit at two different wavelengths, which provides room temperature lasing and detection of two wavelengths monolithically integrated on the same chip.

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[1] B. Schwarz, D. Ristanic, P. Reininger, T. Zederbauer, D.C. MacFarland, H. Detz, A.M. Andrews, W. Schrenk, G. Strasser, "High performance bi-functional quantum cascade laser and detector", Appl. Phys. Lett. 107(7), 071104/1-3 (2015)

[2] A. Harrer, R. Szedlak, B. Schwarz, H. Moser, T. Zederbauer, D. MacFarland, H. Detz, A.M. Andrews, W. Schrenk, B. Lendl, G. Strasser, "Mid-infrared surface transmitting and detecting quantum cascade device for gas-sensing applications", Scientific Reports 6, 21795 (2016)

[3] R. Szedlak, A. Harrer, M. Holzbauer, B. Schwarz , J. Waclawek, D. MacFarland, T. Zederbauer, H. Detz, A.M. Andrews, W. Schrenk, B. Lendl, G. Strasser, "Remote sensing with commutable monolithic laser and detector", ACS Photonics 3(10), 1794–1798 (2016)

Interband cascade ring lasers

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Conference: "Magnetic Excitations in Semiconductors: Bridges to the Next Decade," BUFFALO, N.Y, March 6-8 (2018)

This talk will describe our recent work in the field of interband cascade lasers [1]. Interband cascade lasers are infrared light sources that combine conduction-to-valence band optical transitions with an in-series connection of multiple active regions. Hence, they can be seen as hybrids between conventional laser diodes and quantum cascade lasers. Interband tunneling across a type-II band alignment between InAs and GaSb layers allows carrier recycling and to achieve differential quantum efficiencies above unity. With an external bias a semimetallic band alignment is created, where electrons and holes are generated internally. Interband cascade lasers are power-efficient semiconductor devices that cover the infrared spectral region between 2.8 and 11µm [2,3]. We demonstrate a compact substrate-emitting interband cascade laser with a ring-shaped cavity [4]. The light is out-coupled in vertical direction with a second-order distributed feedback grating. A pulsed threshold current density of 0.75 kA/cm² is measured at 20°C for a device emitting at 3.7µm. Finally, we compare the projected nearfields of interband and intersubband cascade ring lasers. While the quantum cascade laser shows an azimuthal orientation, its interband counterpart features a radial polarization of the nearfield. The difference is caused by the nature of the optical transition. Quantum cascade lasers are subjected to the intersubband selection rule, which favors transverse magnetic polarized light. On the other hand, the recombination of electron and heavy-hole leads to transverse electric polarized light emitted from interband cascade lasers.

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[4] M. Holzbauer *et al.*, Appl. Phys. Lett. **111**, 171101 (2017).

Improvements in Geotechnical, Geological & Earthquake Engineering

by John P. Carter, Member EUAS

Short Biography

John Carter was educated at the University of Sydney and Kings' College, University of London. He graduated in Civil Engineering in 1973, and was awarded a PhD in Geomechanics in 1977, and a higher doctorate (DEng) in 2003, all from the University of Sydney. He was an undergraduate cadet and a graduate engineer with the Electricity Commission of New South Wales and he has held academic appointments at the University of Cambridge, the University of Queensland, the University of Sydney, Cornell University, University of Hong Kong, Technical University Graz, and since 2006 with the University of Newcastle. He was promoted to a personal chair at the University of Sydney in 1990 and appointed as its Challis Professor in Civil Engineering in 1999. From 1989 until 2005 he was the Director of the Centre for Geotechnical Research and from 1995 until 1999 he served as Head of the Department of Civil Engineering. He also served as Associate Dean for Research and Acting Dean of the Faculty of Engineering at the University of Sydney. In 2004 he was elected as Chair of the Academic Board at the University of Sydney, a senior position that placed him as one of the Principal Officers of the university with major responsibilities for academic governance. In February 2006 he took up appointment as the Pro-Vice-Chancellor and Dean of Engineering, Faculty of Engineering and Built Environment at the University of Newcastle, Australia, a position he held until his retirement in April 2013. He is now an emeritus professor at the University of Newcastle. He is a former National Chair of the Australian Geomechanics Society. In 2003 he was elected as a Fellow of the Australian Academy of Technological Sciences and Engineering (FTSE) in recognition of his contributions to engineering research and practice. In January 2006 he was appointed as a Member of the Order of Australia (AM) for his contributions to civil engineering through research into soil and rock mechanics and as an adviser to industry. In 2009 he was elected as a Fellow of the Australian Academy of Science (FAA) in recognition of "his work on computational and experimental geomechanics: prediction of the behaviour of geotechnical structures". In 2012 he was elected as a Fellow of the Australian Institute of Building (FAIB). He is also a Fellow of Engineers Australia (FIEAust).

John Carter has more than 40 years of experience in teaching, research and consulting in civil, geotechnical and offshore engineering. His research interests include analytical and numerical modelling, constitutive modelling of soil and rock, soil-structure interaction, rock mechanics, the behaviour of cemented and uncemented carbonate soils, tunnelling, soft soil engineering and offshore foundations. He has attracted more than AUD29 million in competitive research funding and been associated with development projects attracting additional grants of more than AUD4 million. He is the author of more than four hundred refereed technical papers in geotechnical engineering and engineering mechanics, covering a diverse range of topics from theoretical mechanics to experimental applications. He has consulted widely to industry on a range of geotechnical projects including soft clay foundations, offshore foundations, retaining walls, buried structures and tunnelling. He has also been retained as a consultant on numerous offshore foundation problems for major oil and gas companies, including BHP, Esso, Woodside, Wapet, Bond Oil, Amoco and Exxon. He has acted as an expert witness for courts in NSW, Victoria and Queensland. From 1995 until December 2013 he was a consultant director of Advanced Geomechanics, a geotechnical engineering consultancy based in Perth, Western Australia, providing specialist advice to the oil and gas sector on foundation problems and on-shore and offshore site investigations. He has also been involved in commercialization of research and the marketing of its outcomes, including his own specialist geotechnical software. Between 1997 and 2000 he was a director, representing the interests of the University of Sydney,

of Benthic GeoTech Pty Ltd, a AUD10 million joint venture company that conceived, designed, built and now operates PROD, the Portable Remotely Operated Drill, which is used in water depths out to 2000 m to penetrate the ocean floor in order to conduct in situ tests and recover core samples from the sea floor. He is a former Director and Chairman of UoN Singapore, a controlled entity of the University of Newcastle, responsible for delivering its degree programs in Singapore. In May 2008 he was appointed by the New South Wales State Treasurer as a member of the Board of Newcastle Port Corporation, a position he held until June 2014. He is currently a director of Engineering Aid Australia, a not-for-profit organization that supports and encourages Indigenous Australians to study engineering. In 2009 he became a Graduate Member of the Australian Institute of Company Directors.

Chai, J-C. and Carter, J. P. (2011). Deformation Analysis in Soft Ground Improvement, Springer, Series: Geotechnical, Geological and Earthquake Engineering, Vol. 18, 247p.

First comprehensive text book treatment of the subject area.

ABSTRACT (ABRIDGED): This book describes a variety of analytical and numerical models, based firmly on experimental evidence from observations made in both the laboratory and the field, which can be used in geotechnical engineering to make predictions of soil deformations arising from or associated with ground improvement techniques. The use of such techniques is becoming ever more popular in soft ground engineering. The deformations of the ground addressed in this work are often time-dependent and, given that soft soil behaviour can be highly non-linear, they are often difficult to estimate reliably.

Randolph, M. F., Carter, J. P., Wroth, C. P. (1979). Driven Piles in Clay - The Effects of Installation and Subsequent Consolidation. *Géotechnique,* 29: 361-93.

Seminal paper on the effective stress analysis of the influence of pile installation on the surrounding soil.

ABSTRACT: This paper describes the results of numerical analysis of the effects of installing a driven pile. The geometry of the problem has been simplified by the assumption of plane strain conditions in addition to axial symmetry.
Pile installation has been modelled as the undrained expansion of a cylindrical cavity. The excess pore pressures generated in this process have subsequently been assumed to dissipate by means of outward radial flow of pore water. The consolidation of the soil has been studied using a work-hardening elasto-plastic soil model, which has the unique feature of allowing the strength of the soil to change as the water content changes. Thus it is possible to calculate the new intrinsic soil strength at any stage during consolidation. In particular the long-term shaft capacity of a driven pile may be estimated from the final effective stress state and intrinsic strength of the soil adjacent to the pile. A parametric study has been made of the effect of the past consolidation history of the soil on the stress changes due to installation of the pile. The results indicate that for any initial value of overconsolidation ratio, the final stress state adjacent to the pile is similar to that in a normally one-dimensionally consolidated soil except that the radial stress is the major principal stress. A method is described whereby the model of pile installation and subsequent consolidation may be extended to clays which are sensitive. The method is used to predict changes in the strength and water content of soil adjacent to a driven pile which compare well with measurements from two field tests on driven piles. It is also shown that the rate of increase of bearing capacity of a driven pile may be estimated with

reasonable accuracy from the rate of increase in shear strength of the soil predicted from the analysis.

Carter, J. P., Booker, J. R. and Small, J. C. (1979). The Analysis of Finite Elasto-Plastic Consolidation. *International Journal for Numerical and Analytical Methods in Geomechanics*, 3: 107-129.

First paper to solve large deformation elastoplastic consolidation problems.

ABSTRACT: A theoretical formulation and a numerical solution method are proposed for the problem of the time dependent consolidation of an elasto-plastic soil subject to finite deformations. The soil is assumed to be a two-phase material with a skeleton which may yield according to a general yield criterion with plastic flow governed by a general flow law, and whose pore fluid flows according to Darcy's Law. Governing equations are cast in a rate form and constitutive laws are expressed in a frame indifferent manner. The method of analysis is illustrated by several examples of practical interest for both a soil with an elastic skeleton and a soil with an elasto-plastic skeleton which obeys a Mohr-Coulomb yield criterion and a non-associated flow law.

Carter, J. P., Booker, J. R., Yeung, S. K. (1986). Cavity Expansion in Cohesive Frictional Soils. *Géotechnique*, 36(3): 349-58.

Analytical solution to a classical problem in solid mechanics.

ABSTRACT: Closed form solutions are presented for the expansion of cylindrical and spherical cavities in an ideal, cohesive frictional soil. An explicit solution for the pressure-expansion relationship can be obtained for infinitesimal small strain) deformations. For finite deformations it is necessary to adopt a numerical approach to obtain the complete pressure-expansion relationship and it is found that the cavity pressure approaches a limiting value for infinite deformation. It is, perhaps surprisingly, possible to determine the precise value of this limiting pressure analytically. It is suggested that the small strain solution for a cylindrical cavity is apphcable to the interpretation of pressuremeter tests in sand, and that the solutions for limit pressures have application to the problem of pile installation and the end bearing pressure of deep foundations.

Taiebat, H. and Carter, J. P. (2000). Numerical Studies of the Bearing Capacity of Shallow Footings on Cohesive Soil Subjected to Combined Loading. *Géotechnique*, 50(4): 409-418.

First rigorous solutions to a classical problem in elastoplasticity.

ABSTRACT: This paper presents the results of three-dimensional analyses of circular foundations on the surface of homogeneous, purely cohesive soil. The foundations were assumed to adhere fully to the soil, and compressive, tensile and shear stresses may develop at the interface between the footing and the soil. The predicted ultimate response of the foundations to combined vertical, moment and horizontal loading was compared with other available theoretical predictions. A three-dimensional failure locus is presented for these foundations, based on the numerical predictions. An equation that approximates

the shape of the failure locus is also suggested, and this provides a convenient means of calculating the bearing capacity of circular foundations on a uniform clay and subjected to combined loading.

Liu, M. D., and Carter, J. P. (2002). A Structured Cam Clay Model. *Canadian Geotechnical Journal*, 39(6), 1313-1332.

Presents a relatively simple, practical model for structured clays.

ABSTRACT: A theoretical study of the behaviour of structured soil is presented. A new model, referred to as the Structured Cam Clay model, is formulated by introducing the influence of soil structure into the Modified Cam Clay model. The proposed model is hierarchical, i.e., it is identical to the Modified Cam Clay soil model if a soil has no structure or if its structure is removed by loading. Three new parameters describing the effects of soil structure are introduced, and the results of a parametric study are also presented. The proposed model has been used to predict the behaviour of structured soils in both compression and shearing tests. By making comparisons of predictions with experimental data and by conducting the parametric study it is demonstrated that the new model provides satisfactory qualitative and quantitative modelling of many important features of the behaviour of structured soils.

Carter, J. P. and Booker, J. R. (1982). Elastic Consolidation Around a Deep Circular Tunnel. *International Journal of Solids and Structures* 18 (12), 1059-1074

Rigorous closed-form solutions to a classical problem in tunnelling.

ABSTRACT: A method of analysis is presented for the consolidation of a linear elastic soil due to the cutting of a long and deep circular tunnel. Solutions have been obtained for the time dependent displacements and stress changes occurring in the soil surrounding the tunnel opening.

Nazem, M., Carter, J. P. and Airey, D. W. (2009). Arbitrary Lagrangian-Eulerian Method for Dynamic Analysis of Geotechnical Problems. *Computers and Geotechnics*, 36: 549–557.

Practical solution to a long-pondered problem of overcoming mesh distortion in large deformation finite element analysis.

ABSTRACT: In this paper an arbitrary Lagrangian–Eulerian (ALE) method to solve dynamic problems involving large deformation is presented. This ALE method is based upon the operator-split technique in which the material displacements and mesh displacements are uncoupled. A brief history of the ALE method is first presented and then special issues such as time-stepping, mesh refinement, energy absorbing boundaries, dynamic equilibrium checks and remapping of state variables are explained. The ALE method and the updated-Lagrangian (UL) method are then used to analyse some geotechnical problems to examine the significance of inertia effects, large deformation and contact mechanics. The results show the efficiency of the ALE method for solving dynamic geotechnical problems involving large deformation.

Taiebat, H., and Carter, J. P. (2002). Bearing Capacity of Strip and Circular Foundations on Undrained Clays Subjected to Eccentric Loads. *Géotechnique*, 52(1): 61-64.

Rigorous plasticity solutions to a classical problem in foundation engineering.

ABSTRACT: The objective of the current studies is to determine the shape of the failure locus for shallow strip and circular foundations in (**V**, **M**) space using the results of a finite element study of this problem. (**V** = applied vertical load, **M** = applied moment). The (**V**, **M**) load case is significant, as it also corresponds to footing problems in which the vertical load is eccentrically applied.

Nazem, M., Carter J. P., Airey, D.W. and Chow, S.H, (2012) Dynamic analysis of a smooth penetrometer free-falling into uniform clay, *Géotechnique*, 62(10): 893-905.

First solution to a dynamic penetration problem in soil. Awarded the Manby Prize by the Institution of Civil Engineers, London.

ABSTRACT: The finite-element analysis of free-falling objects penetrating soil deposits is one of the most sophisticated and challenging problems in geomechanics. A robust numerical method will be described here for dealing with such complex and difficult problems. The approach is based on the arbitrary Lagrangian–Eulerian (ALE) method of analysis, the main features and challenges of which are described briefly in the paper. The ALE method is then employed to perform a parametric study of a perfectly smooth penetrometer free-falling into a uniform layer of clay, which deforms under undrained conditions. The effect of the mechanical properties of the clay soil on the penetration characteristics is presented, and an approximate, closed-form expression is derived for the dynamic penetration factor, $\mathbf{N}_{dp}$: Comparisons are made between the deduced values of $\mathbf{N}_{dp}$ and published values of the conventional cone factor, $\mathbf{N}_c$, and comparisons are made with experimental data to validate the approach.

Research in Microbiology, Immunology & Molecular Genetics

by Sherie L. Morrison, Member EUAS

Short Biography

Name: *Sherie L. Morrison, Ph.D.*

Present Title: Distinguished Professor,
Department of Microbiology, Immunology and Molecular Genetics
Member, the Molecular Biology Institute
University of California at Los Angeles

Born: *New Eagle, Pennsylvania - July 5, 1942*

Education:
1959-1963 *B.A. with Distinction and Departmental Honors*
Stanford University, Stanford, California
1963-1966 *Ph.D. Stanford University, Stanford, California*

Recent Honors:
2016 *Recipient of the 2016 Award for I3T Excellence*
2017 *Creation of the Sherie L. Morrison Professorship at Columbia University, Dept. of Microbiology & Immunology, College of Physicians and Surgeons*

Recent Publications:

1. Vasuthasawat, A., Yoo, E. M., Trinh, K. R., Lichtenstein, A., Timmerman, J. M., Morrison, S. L., Targeted immunotherapy using anti-CD138-interferon α fusion proteins and bortezomib results in synergistic protection against multiple myeloma. MAbs. 2016 Jun 30:0. [Epub ahead of print] PMID: 27362935.

2. Li, Z., Zhu, Y, Li, C, Trinh, T, Ren, X, Sun, F., Wang, Y., Shang, P., Wang, T., Wang, M, Morrison, S. L., Zhang, J. Anti-VEGRF2-IFNα2 regulates the tumor microenvironment and exhibits potent anti-tumor efficacy against colorectal cancer, OncoImmunology, 2017.

3. Pushkarsky, I. , Tseng, P, Black, D., France, B., Warfe, L, Koziol-White, C. J., Jester, W. F. Jr., Trinh, R. K., Lin, J., Scumpia, P. O., Morrison, S. L., Panettieri, R. A., Damoiseaux, R., Di Carlo, D., Elastomeric sensor surfaces for high-throughput single-cell force cytometry, Nature Biomedical Engineering 2:124-137, 2018.

4. Trinh, K.R., Vasuthasawat, A., King, R. Y., Timmerman, J. M., Morrison, S. L. Synergistic Inhibition of Multiple Myeloma Growth by Anti-CD138-Interferon –alpha 14 Fusion Protein and Lenalidomide, J. Mol. Immunol, 2018.

5. Young, P.A., Yamada, R. E., Trinh, K.R., Vasuthasawat, A., De Oliveira, S., Yamada, D. H., Morrison, S. L., Timmerman, J. M. Activity of Anti-CD19 Chimeric Antigen

Receptor T Cells Against B Cell Lymphoma Is Enhanced by Antibody-Targeted Interferon-Alpha, J. Interferon & Cytokine Research, 38:239, 2018.

Research

Activity of anti-CD19 CAR T cells against B cell lymphoma is enhanced by antibody-targeted interferon-alpha

Abstract

An important emerging form of immunotherapy targeting B cell malignancies is chimeric antigen receptor (CAR) T cell therapy. Despite encouraging response rates of anti-CD19 CAR T cell therapy in B cell lymphomas, limited durability of response necessitates further study to potentiate CAR T cell efficacy. Antibody-targeted interferon (IFN) therapy is a novel approach in immunotherapy. Given the ability of IFNs to promote T cell activation and survival, target cell recognition, and cytotoxicity we asked whether antibody-targeted IFN could enhance the antitumor effects of anti-CD19 CAR T cells. We produced an anti-CD20-IFN fusion protein containing the potent type I IFN isoform alpha14 (α14), and demonstrated its ability to suppress proliferation and induce apoptosis of human B cell lymphomas. Indeed, with the combination of anti-CD20-hIFNα14 and CAR T cells, we found enhanced cell killing among B cell lymphoma lines. Importantly, for all cell lines pretreated with anti-CD20-hIFNα14, the subsequent cytokine production by CAR T cells was markedly increased regardless of the degree of cell killing. Thus, several activities of CD19 CAR T cells were enhanced in the presence of anti-CD20-hIFNα14. These data suggest that antibody-targeted IFN may be an important novel approach to improving the efficacy of CAR T cell therapy.

Synergistic inhibition of multiple myeloma growth by anti-CD138-interferon-alpha14 fusion protein and lenalidomide

Abstract

Although recent advances have improved the management of multiple myeloma, it remains an incurable malignancy. We now demonstrate that anti-CD138 genetically fused to interferon alpha14 (IFNα14) synergizes with the approved therapeutic lenalidomide in arresting the proliferation of the human multiple myeloma cell line NCI-H929 both *in vitro* and *in vivo*. This synergism is the consequence of the combined effects of multiple, complementary anti-tumor activities including potentiated activation of STAT1 and downregulation of c-Myc, interferon regulatory factor 4 (IRF4) and poly(ADP-ribose) polymerase 1 (PARP-1). Caspase activation and glucose utilization also play a role in the induction of apoptosis by lenalidomide + anti-CD138-IFNα14 as inhibition of caspase activation, glycolysis or oxidative phosphorylation (OXPHOS) decreased but did not eliminate the apoptosis seen following treatment. Treatment with lenalidomide + anti-CD138-IFNα14 results in replicative stress resulting from increased accumulation of reactive oxygen species (ROS). Unexpectedly, we observed that the cellular stress elicited by treatment with lenalidomide or lenalidomide + anti-CD138-IFNα14 results in the degradation of Chk1, the Ser/Thr kinase central to the genome surveillance pathways of the DNA damage response and cell cycle checkpoints. Using an *in vivo* xenograft model we

found that treatment with anti-CD138-IFNα14 + lenalidomide was much more effective than either treatment alone with approximately 40% (9/24) of the animals with established tumors cured. Based on our findings, clinical testing of combination therapy with lenalidomide and anti-CD138-IFN fusion proteins for the treatment of multiple myeloma may be merited.

Imaging Antiferromagnetic Domains: New Trends in Antiferromagnetic Spintronics

by Hartmut Zabel, Member EUAS

Short Biography

After receiving 1978 his Ph.D. in Physics from the Ludwig-Maximilian University of Munich, Hartmut Zabel spent a postdoctoral year at the Department of Physics in Houston, Texas, before joining the faculty of the University of Illinois at Urbana-Champaign in 1979 as Assistant Professor. He was promoted to Associate Professor in 1983 and Full Professor of Physics in 1986. After receiving an offer as Chair of Experimental Physics at the Ruhr-University he moved to Bochum, Germany, in 1989 and established a laboratory in the field of nanomagnetism. Following his retirement in 2013, he became Senior Guest Research Professor at the Universities of Mainz, Germany, and Uppsala, Sweden. Hartmut Zabel has been advisor and co-adviser of 51 PhD students. He is author and co-author of more than 500 research articles published in international scientific journals with more than 12 000 citations, he published more than 30 review papers and book chapters as well as edited and authored 8 books, including an undergraduate textbook on "Medical Physics" (first edition 2017). Hartmut Zabel was named fellow of the American Physical Society in 1996; he received the honorary doctoral degree from the KTH Stockholm in 2001, and the MAINZ Research Award in 2013.

1. Ferromagnetic Spintronics

The discovery of the giant magnetoresistance by Peter Grünberg and Albert Fert in 1988, awarded with the Nobel Prize for Physics in 2007, initiated an upsurge of experimental and theoretical investigations on spin dependent electric transport phenomena. Since then spin valves were introduced, magnetic domain switching via spin-orbit torque was proposed and confirmed, the tunneling magneto-resistance effect has matured to marketability, and magnetic domain walls and their propagation were developed for memory storage devices with enhanced density. This field, which embraces spin-structures and spin-transport in ferromagnets on the nanoscale, was coined spin electronics or short spintronics. Spintronics has become part of everyday technology in form of hard disk data storage media and non-volatile random access memory and is reviewed in Reference [1].

2. Antiferromagnetic Spintronics

More recently the field of antiferromagnetic spintronics promises new opportunities for ultrafast switching. In antiferromagnetic spintronics, ferromagnetic atomic layers are replaced by antiferromagnetic layers as active device materials [2–6]. This approach takes advantage of the ultrafast Tera-Hertz dynamics of antiferromagnets, which is driven by exchange interaction between the ions of opposite spins. This, in principle, enables writing speeds superior to those in conventional ferromagnetic spintronic devices. Moreover, the absence of a net magnetization in antiferromagnetic materials results in vanishing dipolar magnetic interactions, allowing, in principle, for an increased information density and a high stability against disturbing external fields. In antiferromagnetic spintronics, information is encoded by the direction of the Néel vector, which is defined by the vector difference of the sublattice magnetizations. For spintronic applications, one requires

efficient methods for reading the Néel vector orientation and changing its orientation for writing. In case of antiferromagnets with non-centrosymmetric magnetic sublattices, it was predicted that a current-induced spin-orbit torque can change the orientation of the Néel vector [7]. This was indeed recently demonstrated for the some antiferromagnetic compounds [8-11]. However, the necessary current densities are, in general, close to the destruction limit and further materials optimization is required. Therefore, the characterization of antiferromagnetic domain structures in relevant materials is of major importance. Before going into further details, we first reflect on the existence and characteristics of magnetic domains in ferro- and antiferromagnetic materials and how they can be visualized.

3. Magnetic Domains

Single domain ferromagnets are surrounded by a dipolar magnetic field connecting north pole and south pole as shown in Fig. 1(a). The dipolar magnetic field is technically useful for lifting metals or keeping charged particles on their track in particle accelerators, but they are energetically unfavorable. Therefore, ferromagnets tend to form macroscopic magnetic domains in order to reduce the energy that is stored in the dipolar magnetic field. This is schematically illustrated in panels (b)-(e). In panels (b) and (c) we notice magnetic domains with alternating magnetization direction and 180° domain walls in-between. At the top and bottom edge domains may develop with 90° domain walls with respect to the elongated domains as shown in panels (d) and (e). Creating domains costs energy, so called exchange energy, and therefore the final domain structure results from a balance of exchange energy and magneto-crystalline energy, while the dipolar field energy is nulled. Furthermore, magnetic domains are usually separated by straight domain walls and the magnetization within the domains points along the easy magnetization direction determined by the magneto-crystalline anisotropy.

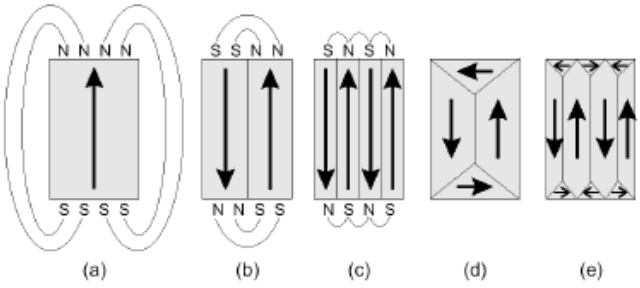

Fig. 1 - Magnetic domains in ferromagnetic materials: (a) single domain. (b)-(e) creating more domains reduces the dipolar field outside. Reproduced from [11].

Antiferromagnets do not exhibit dipolar magnetic fields. Due to the antiparallel spin orientation on the atomic scale, dipolar fields are compensated locally. Antiferromagnets are non-magnetic from a macroscopic point of view and are difficult to recognize as being magnetic on an atomic scale. Therefore, one should conclude that antiferromagnets do not exhibit domains. However, fact is that antiferromagnets also exhibit magnetic domains. They are much harder to reveal, but they do exist. The question is why? And if antiferromagnetic domains exist, what determines there size, the orientation of the Néel vector within the domains, and the domain wall width? There are no simple answers to these questions. It is generally believed that the existence of antiferromagnetic domains is due to entropy. Creation of domains increases the disorder in antiferromagnetic spin structures thereby increasing the entropy S and lowering the Gibbs free energy G

according to $\Delta G = \Delta U - T\Delta S$, where U is the internal energy and T is the absolute temperature. Furthermore, antiferromagnetic spin order, unlike ferromagnetic order, relies on the perfection of the underlying crystallographic structure. Line defects such as edge or screw dislocations are likely to disturb the antiferromagnetic spin structure as much as they disturb the ionic structure of a crystal lattice. Finally, as antiferromagnets lack contributions from the dipolar magnetic field to the total free energy, even small contributions from the magneto-crystalline anisotropy may become relevant. The magneto-crystalline anisotropy usually is coupled to a magneto-elastic anisotropy that distorts the crystal lattice according to the spin orientation within a domain. Then the total elasto-mechanical energy can be lowered by a checkerboard arrangment of antiferromangetic domains, as shown schematically in Fig. 2. Which one of these three effects (entropy, crystal defects, and magneto-elastic anisotropy) is finally responsible for the existence of antiferromagnetic domains remains to be seen but most likely depends on the specific antiferromagnetic material.

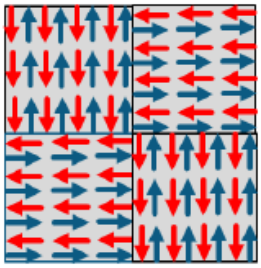

Fig. 2 – Magnetic domains in antiferromagnets.

4. Magnetic Domain Imaging

Imaging ferromagnetic domains is comparatively easy. Early imaging experiments were carried out with iron powder dispersed across the surface of a ferromagnet like spreading salt or papper. However, the spatial resolution is rather low. Todays more advanced experimental techniques use either magnetic force microscopy or optical based methods via laser light, electron microscopy, synchrotron radiation or thermal neutron beams. One particular powerful method is the so-called x-ray photo-electron emission microscopy (X-PEEM). X-PEEM uses the photoelectric effect with incident x-rays tuned to an absorption edge of an element in the ferromagnetic material, such as the L-edge of Fe or Co. The emitted photo-electrons are extracted by a potential gradient and go through an electric lens system like in an electron microscope and finally impinge on a photoplate or CCD chip for imaging. With this arrangement, spatial resolution of about 20 nm has been reached. To attain magnetic sensitivity and deliver conrast for different domain orientations, the incident x-ray beam must - in addition - be circularly right (+) or left (-) polarized. Magnetic contrast is then achieved by the contrast of the absorption coefficents $\mu_{+,-}$ for both circular polarizations: $\Delta\mu=\mu_{+}-\mu_{-}$. The reason for the contrast is the difference in the electron density of states at the Fermi level for up- and down polarized electrons. This imaging method is accordingly coined x-ray circular magnetic dichroism-PEEM or XMCD – PEEM. Fig. 4 shows an XMCD-PEEM image of two antiparallel magnetic domains in a thin Co-film.

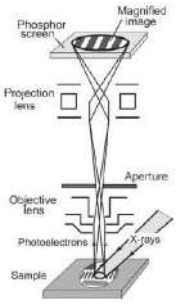

Fig. 3 - Schematic outline of electron optics in an X-PEEM instrument. From [12].

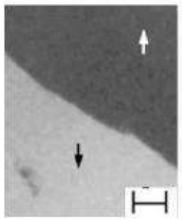

Fig. 4 - Magnetic domains in a ferro-magnetic Co-film, imaged by XMCD – PEEM. The scale bar corresponds to 10 μm. From [13].

What works well for ferromagnets does not offer a solution to imaging domains in antiferromagnetic materials. In antiferromagnets the electron density of states is not split at the Fermi-level and therefore no magnetic circular dichroism exists. However, using linear polarization, a slight difference exists in the absorption spectrum close to the L-edge for the x-ray electric field vector being oriented parallel or perpenduclar to the antiferromagnetic spins. This tiny difference that is seen in metallic antiferromagnets can be used for imaging antiferromagnetic domains, the method is referred to as XMLD-PEEM.

5. Magnetic Domains in Antiferromagnetic Mn_2Au

For switching antiferromagnetic domains by electric current, the material should exhibit metallic properties. There are only a few materials available that feature both metallic conductivity and antiferromagnetic order at room temperature. Among those are the alloys CuMnAs and Mn_2Au which are presently discussed most intensively for potential antiferromagnetic spintronics [8-10]. As detailed above, before considering any device application, the antiferromagnetic domain structure needs to be known. We have unraveled the domain structure before and after applying extremely high magnetic fields via XMLD-PEEM imaging methods, using a microscope installed at the synchrotron facility BESSY II of the Hemlholtz-Zentrum Berlin. Results are shown in Fig. 5 for an as-deposited thin film of epitaxially grown Mn_2Au and before applying a magnetic field. Antiferromagnetic domains are visible in panel (a) and are confirmed by a one-to-one correspondance of contrast switch after rotating the electric field vector by 90°, as indicated by the red arrow. These images show that antiferromagnetic domains exist in Mn_2Au films, that the magnetic domain size is approximately 1μm and that the domain walls are irregularly oriented with a width well below 1 μm. In fact, the domain wall width was estimated to be about 50 nm. These antiferromagnetic domains can be manipulated by an external magnetic field. But the spin-flop field where the spins change orientation is beyond 30 T, not convenient for application. Therefore, switching domains by electric currents remains a promising option.

In conclusion, using XMLD-PEEM, we succeeded in imaging domains in

antiferromagnetic Mn_2Au thin-film samples. Their sizes are approximately 1 μm. The domain wall width is below 80 nm and exhibits an irregular shape. Antiferromagnetic domains in Mn_2Au can be manipulated by a large magnetic field of 30 T and beyond, generating a spin-flop transition.

This contribution is based on the publication "Direct imaging of antiferromagnetic domains in Mn_2Au manipulated by high magnetic fields", authored by A. A. Sapozhnik, M. Filianina, S. Yu. Bodnar, A. Lamirand, M.-A. Mawass, Y. Skourski, H.-J. Elmers, H. Zabel, M. Kläui, and M. Jourdan, which was published in Physical Review B 97, 134429 (2018).

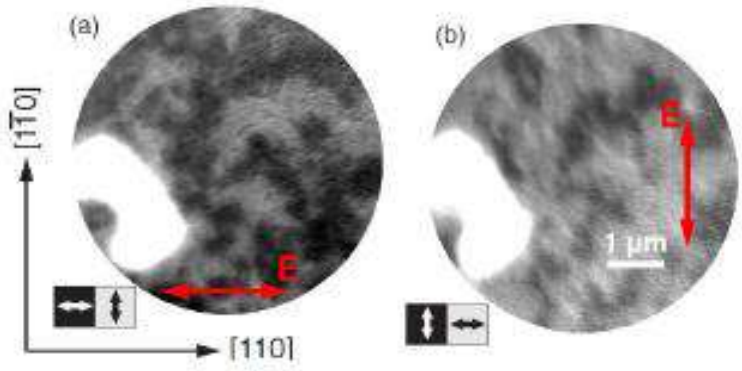

Fig. 5 - Antiferromagnetic domains in a Mn_2Au film imaged by XMLD-PEEM. (a) E-vector parallel to spins; (b) E-vector perpendicular to spins. From [14].

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New Methods using Remote Sensing and GIS for Cartography and Environment

by Manfred F. Buchroithner EUAS

Short Biography

Manfred Ferdinand Buchroithner (17-12-1950) studied Geology & Palaeontology at the University of Graz/Austria and both Remote Sensing and Cartography at ITC/Nederlands. He obtained his PhD in 1977 in Graz. In 1982 he went as Fulbright Scholar to the USA (Fort Worth/Texas, Boulder/Colorado and Stanford University/California). During the following years at the Institute for Cartography of the Austrian Academy of Sciences in Vienna and as Director of the Joanneum Research Institute of Digital Image Processing and Computer Graphics in Graz he spent several months of postdoctoral research at the Finnish National Research Center/VTT in Espoo near Helsinki and at the Jet Propulsion Laboratory/JPL of NASA in Pasadena. In 1985 he obtained his habilitation (venia legendi) for both General Geology and Remote Sensing. From 1992 to 2016 he was Full Professor holding the Chair of Cartography at TU Dresden, Germany. He obtained several scientific awards and is member of several learned societies.*

The First Depiction of Two Superimposed Geographical Surfaces in One Autostereoscopic Map: Antarctica's Topography and the Southern Ocean Seafloor

Manfred F. Buchroithner and Lars Radig

THE CARTOGRAPHIC JOURNAL 2018, VOL. 55, NO. 1, pp. 58-67

Abstract

Within the past 10-15 years true-30 lenticular cartography has experienced a remarkable boost. ln the course of this development, besides studies into its potential for thematic-cartographic representations, the synoptic depiction of physical surfaces Cgeo[graphical] surfaces) has been playing a significant role. ln this context the innovative holistic display of complex morphological and topographical conditions is of particular interest. The simultaneaus representation of various cartographic parameters at different depths will deliver an enormous surplus of information transfer in the field of thematic cartography as weil as in physical/topographic cartography. This paper describes the methodological development and generation of an autostereoscopic hardcopy display of Antarctic topography. The purpose was the simultaneaus depiction of the two superimposed surfaces of both the ice- sheet and the rock-bed and, in addition, of the surrounding seafloor, thus displaying a vertical drop of more than 12,000 m.

Above-ground biomass estimation based on NPP time-series – A novel approach for biomass estimation in semi-arid Kazakhstan

Christina Eisfelder, Igor Klein , Aruzhan Bekkuliyeva , Claudia Kuenzer , Manfred F. Buchroithner, Stefan Dech

ECOLOGICAL INDICATORS 72(2017), 13-22

Abstract

Biomass is a sensitive indicator of environmental change and ecological functioning. Quantification of biomass is essential to identify and monitor those areas threatened by degradation and desertification. This is especially important in arid and semi-arid environments. However, robust techniques to monitor carbon stocks over Iarge areas and through time are still missing. The major objective of the presented study is to develop a novel approach for biomass estimation in semi-arid environments using remote- sensing based Net Primary Productivity (NPP) data.

The developed methodical concept aims at derivation of above-ground grass and shrub biomass for natural environments. 1t is based on NPP time-series and plants' relative growth rates. Fractional cover data provide information about grass and shrub coverage. The developed approach has been applied to three study areas in Kazakhstan, in which field data were collected for validation.

Biomass maps were derived that show the spatial distribution of grass and shrub biomass. Validation revealed a moderate correlation (R=0.68) with field data for grass biomass. For shrub biomass, a high correlation (R = 0.83) is retrieved when fractional cover information from field Observations is used.

The presented novel approach for biomass estimation is based on remote sensing derived NPP time- sedes and is thus potentially transferable in space and time. This is a great advantage compared to commonly applied empirical relationships. The presented concept can be adapted to be applied to other vegetation communities. Providing the necessary data about fractional vegetation cover is available, the method will allow for repeated and large-area biomass estimation for natural semi-arid environments as needed for observing changes in biomass and support sustainable land management.

New insights on permafrost genesis and conservation in talus slopes based on observations at Flüelapass, Eastern Switzerland

Robert Kenner, Marcia Phillips, Christian Hauck, Christin Hilbich, Christian Mulsow, Yves Bühler, Andreas Stoffel, Manfred Buchroithner

Geomorphology 290 (2017) 101-113

Abstract

The talus slope at Flüelapass was the first mountain permafrost study site in Switzerland in the 1970s and the presence of ice-rich permafrost at the foot of the slope has been investigated in the context of several studies focusing on the roJe of snow cover distribution. We review previously developed hypotheses and present new ones using various data sources, such as temperature measurements in boreholes, a subaquatic DEM

generated from unmanned aerial system (UAS) photogrammetry, terrestrial Iaser scan measurements of snow depth, geophysical ground investigations and automatic time-Japse photography. From this combination of data sources tagether with Observations in the field, an interesting sequence of geomorphologic processes is established at Flüelapass. As a result we show how mass wasting processes can initiate the genesis and long-term conservation of ice-rich permafrost at the base of a talus slope.

Combining Partial Least Squares and the Gradient-Boosting Method for Soil Property Retrieval Using Visible Near-Infrared Shortwave Infrared Spectra

Lanfa Liu, Min Ji and Manfred Buchroithner

Remote Sensing 9 (2017), 1299

Abstract

Soil spectroscopy has experienced a tremendous increase in soil property characterisation, and can be used not only in the laboratory but also from the space (imaging spectroscopy). Partial least squares (PLS) regression is one of the most common approaches for the calibration of soil properties using soil spectra. Besides functioning as a calibration method, PLS can also be used as a dimension reduction tool, which has scarcely been studied in soil spectroscopy. PLS components retained from high-dimensional spectral data can further be explored with the gradient-boosted decision tree (GBDT) method. Three soil sample categories were extracted from the Land Use/Land Cover Area Frame Survey (LUCAS) soillibrary according to the type of land cover (woodland, grassland, and cropland). First, PLS regression and GBDT were separately applied to build the spectroscopic models for soil organic carbon (OC), total nitrogen content (N), and clay for each soil category. Then, PLS-derived components were used as input variables for the GBDT model. The results demonstrate that the combined PLS-GBDT approach has better performance than PLS or GBDT alone. The relative important variables for soil property estimation revealed by the proposed method demonstrated that the PLS method is a useful dimension reduction tool for soil spectra to retain target-related information.

Deterministically Defining Chambers in 3D-Scans of Caves

Nico Schertlerl, Manfred Buchroithner, Donald McFarlane, Guyvan Rentergem, Joyce Lundberg, Stefan Gumhold

Proceedings ofthe 17th International Congress of Speleology

Abstract

Increasingly, speleologists are employing terrestriallaser scanners to generate highly detailed 3D maps of caves, which can be used for quantitative analysis and comparison. Although their high precision allows very accurate volume computations, one of the key aspects of cave mapping- the identification of chambers for volumetric camparisans-still remains a manual post-processing step. Naturally, such manual steps are heavily influenced by subjective preferencesandnot suited for objective comparisons. In this paper, we present a novel algorithm that bridges this gap. Given an appropriate 3D model of a cave, our algorithm produces a unique and unambiguous segmentation of the cave into distinct chambers and passages. It is free ofhuman bias andinsensitive to scanning noise, scaling, and orientation of the model. The foundation of our work is a thorough analysis of cave geometry. We transfer the results of this analysis into a mathematical modeland use state-of-the-art methods from computer graphics to derive the segmentation. We initially tested our approach with various cave models and a group of speleologists, which confirmed that our algorithm's results conform closely to manual segmentations. Therefore, it seems to be well-suited as a substitute for "classical" but ambiguous existing approaches to comparing chamber volumes, and can provide objective comparability to the process.

Chamber Recognition in Cave Data Sets

Nico Schertler, Manfred Buchroithner and Stefan Gumhold

EUROGRAPHICS 36 (2017)

Abstract

Qunntitative aMlysis of cave systems represented as 3D models is becoming more and more important in the fold of cave sciences. One open question is the rigorous identification of chambers in a data set, which has a deep impact on subsequent aMlysis steps such as size calculation.This affects the inteTMtioMl recognition of a cave since especially record-holding caves bear significant tourist attraction potential. In the past, chambers have been identified manually, without any clear definition or guidance.While experts agree on core parts of chambers in general, their opinions may differ in more controversial areas. Since this process is heavily subjective, it is not suited for objective quantitative comparison of caves. Therefore, we present a novel fully-automatic curve skeleton-based chamber recognition algorithm that has been derived from requirements from fold experts.We state the problern as a binary labeling problern on a curve slceleton and find a solution through energy minimization. A tharough evaluation of our results with the help of expert feedbaclc showed that our algorithm matches real-world requirements very closely and is thus suitedas the foundation for any quantitative cave aMlysis system.

Functionalized Nanomaterials for Energy and Biomedical Applications

by Yuehe Lin, Member EUAS

Short Biography

Dr. Yuehe Lin is a professor in the School of Mechanical and Materials Engineering, School of Chemical Engineering and Bioengineering, and the Paul G. Allen School for Global Animal Health at Washington State University (WSU). He also holds a joint appointment at Pacific Northwest National Laboratory (PNNL), conducts research in nanotechnology, particularly development of small-scale devices, nanomaterials and analytical systems for biomedical diagnosis, drug delivery, energy and environmental applications. Dr. Lin joined PNNL in 1997 first as a post-doctoral fellow and then as a full-time research scientist in 1998. He was promoted to Senior Research Scientist in 2000 and Chief Scientist in 2004. In 2008, Dr. Lin was named a Laboratory Fellow, the highest rank in DOE national laboratory system. He joined WSU in 2013 as a full professor in the School of Mechanical and Materials Engineering, School of Chemical Engineering and Bioengineering, and the Paul G. Allen School for Global Animal Health.

Dr. Lin's research has been funded by NIH, CDC, USDA, DOE, and DOD with a total budget over $25M for a total of 30 projects. His research has resulted in about 460 publications with a total citation of 46,000 and h-index 110. He was listed in Thomson Reuters's highly-cited researchers in 2014, 2015, 2016, 2017 and 2018. Dr. Lin is a fellow of American Association for the Advancement of Science (AAAS), Royal Society of Chemistry (RSC) and American Institute of Medical and Biological Engineering (AIMBE). He is a member of EUAS and Washington State Academy of Sciences (WSAS). He currently hold 20 patents. Some of the patents have been licensed to industrial partners for commercialization. He obtained Battelle-PNNL Key Contributor Awards three times for successful technology commercialization. He serves as the editor of Analytica Chimica Acta and editorial board members of ~ 20 international journals such as Biosensors and Bioelectronics, Electroanalysis, Sensors and Actuator B, International Journal of Nanomedicine, Advance Materials Technologies.

Dr. Lin is also an effective mentor and educator. During his entire career at PNNL and WSU, he has supervised many undergraduate and graduate students in his lab, including 10 undergraduate students and over 16 Ph.D. students and 20 postdocs. In past three years, three of his Ph.D. students received the Excellent Research Awards, two in Materials Science and Engineering Program (2016, 2017; one person each year) and one in Mechanical Engineering. More than 30 of his students, postdocs and visiting scholars have become successful professors, scientists and engineers at national laboratory, universities and industrial companies.

Dr. Lin's work focus on synthesis of functional materials and their applications in biotechnology, medicine, environment and energy. Some of his major contribution to the materials science and engineering are briefly summarized in the following:

1. Synthesis and characterization of nanoscale materials

Dr. Lin's recent work in this area includes the synthesis of nanoparticles and nanowires using supercritical fluid processing, chemical reduction, and electrochemical methods. Electro-synthesis of nanowires through both template and templateless approaches. Synthesis of electrocatalysts based on nano-carbon supports (e.g. mesoporous carbon, carbon nanotubes, graphene) for fuel cell, water splitting, and other energy & environmental applications. The work in this area has resulted in a list of high-impact publications in *Advanced Materials* 2003, 15(4), 316-319 (highly cited); *Angewandte Chemie International Edition* 2002, 41(19), 3665-3668 (highly cited); *Journal of the American Chemical Society* 2011, 21(14), 5319-5325; *Advanced Materials* 2016, 28, 8779-8783; *Advanced Energy Materials* 2017, 7, 1601555 and 2018, 8, 1801956 and several patents.

2. Lab-on-chip/Microtechnology/3D printing/smartphone based biosensors

Dr. Lin's group have developed the miniaturized analytical devices based on integration of the capillary electrophoresis-microchip with an electrochemical detector for detecting biomolecules, explosives, and nerve agents. A portable analytical system based on the integration of a microfluidic motherboard with a microelectrode array was developed for biomonitoring of toxic chemicals in biological samples. Various microtechnology-based microdevices, using laser-microfabrication technology have also been fabricated at his lab. The microdevices have been successfully used in sample process of biological samples for mass spectrometry/proteomics. The research resulted in a list of high-impact publications and several patents. The microtechnology-based sample processing devices has been licensed to several industrial partners for commercialization.

Recently, Dr Lin's group have developed paper-based biosensing devices and 3D printed devices, in combination with smartphone for point-of care and on-site detection, and applied these portable platforms in biomedical diagnosis and food safety monitoring (*Analytical Chemistry* 2018, 90 (12), 7391-7398; *Biosensors & Bioelectronics* 2018, 104, 39-44 and *ACS Applied Materials & Interfaces* 2017, 9, 40671-40680).

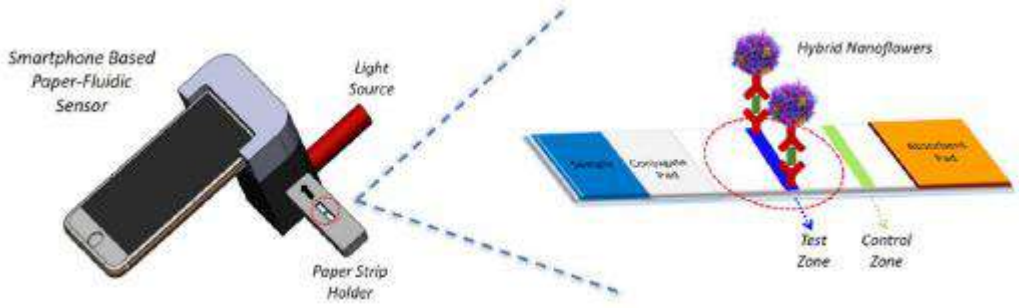

Figure 1 3D Printed portable analytical system with a smartphone reader.

3. Nanostructured electrochemical sensors and biosensors

Because of their size, nanoscale materials have different chemical and physical properties than their bulk counterparts and thus, behave differently. One of these properties is the ability to be "functionalized" or custom-designed to attract specific molecules. Another property is an extremely high surface area. The unique characteristics of nanoscale materials make them a perfect fit for sensors. Dr. Lin's lab has done some pioneering work in this area. His papers on functionalization of carbon nanotubes for biosensing published in the *Journal of the American Chemical Society* (2003, 125(9), 2408-2409) has received ~1500 citations, *Electrochemical Communications* (2002, 4, 743-746) has received ~1300 citations. He and his collaborators have developed different kinds

of biosensors based on carbon nanotube nanoelectrode arrays (CNT-NEAs). Consisting of millions of individual nanoelectrode with diameter of 100 nm, the NEAs were made in 1 cm^2 area by this non-lithography method. The key issue is controlling the density of the nanoelectrode array to prevent the overlap of diffusion layers. By controlling density, nanoelectrode array maintained nanoelectrode property, leading to >3 orders of magnitude improvement in S/N ratio. One patent was issued and several publications on *Nano Letters* (2003, 3(1), 107-109 and 2004, 4(2), 191-195), and *Analytical Chemistry* (2006, 78(21), 7417-7423) are highly cited in the field.

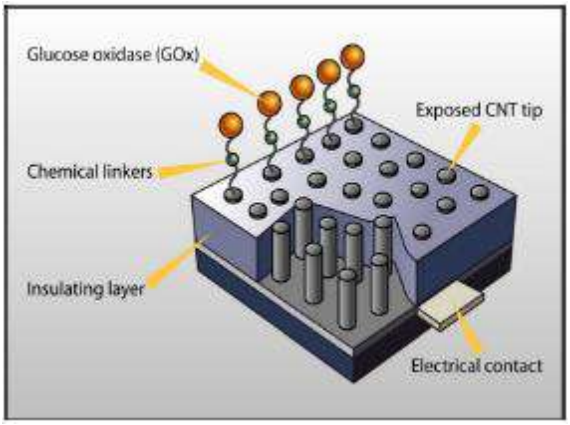

Figure 2 Biosensors based on carbon nanotube nanoelectrode arrays.

4. Functionalization of graphene for biosensing and bioimaging

Recently, Dr. Lin's group has pioneered the work in graphene and 2D materials-based biosensors and bioimaging. His group have synthesized graphene, graphene oxides and other 2D materials (C_3N_4, MnO_2) and functionalized them with DNA, apatmers, enzymes and antibodies for biosensing and bioimaging applications. Their pioneered works have been published in top journals and received very good citations. For example, Dr. Lin was invited to write the first review article on this topic (*Electroanalysis* 2010, 22(10), 1027-1036, citation ~2300). Graphene-based enzyme biosensors is one of the most-cited papers in the *ACS Nano* 2010, 4, 1790-1798 with 1600 citations, and *Biosensors & Bioelectronics* 2009, 25(4), 901-905 with ~1000 citations. DNA and aptamer based graphene probes have been developed for detection of DNA (*Small* 2010, 6(11), 1205-1209, journal cover) and for cell imaging (*Journal of the American Chemical Society* 2010, 132(27), 9274-9276, 850 citations). Graphene-based immunosensors have been developed for detection of cancer biomarkers (*Analytical Chemistry* 2010, 82(7), 2989-2995 and 2011, 83(3), 746-752).

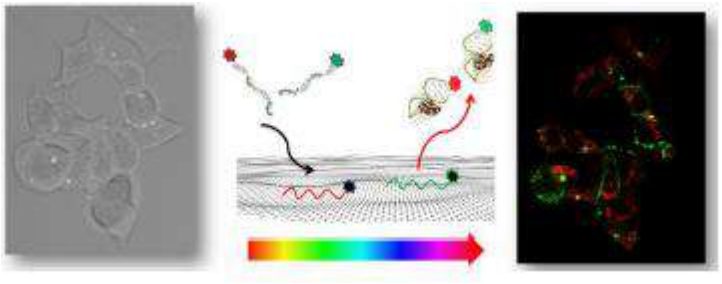

Figure 3 Aptamers/graphene oxide nanosheets for simultaneous probe ATP and GTP in living cell.

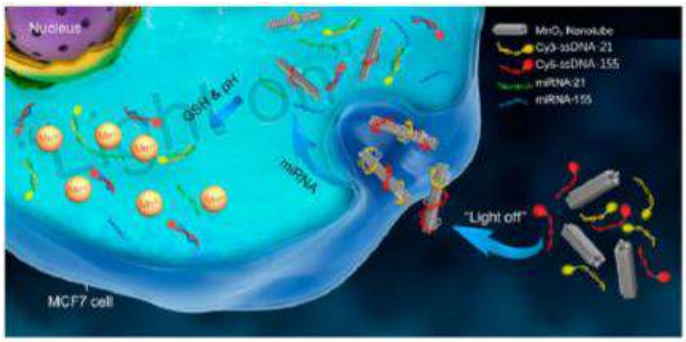

Figure 4 MnO2 nanotubes for imaging of multiple micrornas in living cells.

5. Nanoparticle labels for immunoassay and DNA assays, imaging and drug delivery

Dr. Lin's group have synthesized the biotemplated nanomaterials and mesoporous SiO_2 nanoparticles for bio-functionalization and biosensing. The major barriers for applications of quantum dots/metal nanoparticles for imaging/diagnostics applications are the instability and toxicity (for in vivo imaging) of the quantum dots. His laboratory has synthesized various protein-cage based nanoparticles and demonstrated sensitive detection of DNA and protein biomarkers. Recently, protein-cage for drug delivery for nuclear medicine was demonstrated. These works could lead to the next-generation biosensing devices and drug delivery for early diagnostics and treatment of different diseases. The works in this area have resulted in a list of high-impact publications (*Journal of the American Chemical Society* 2007, 129(34), 10394-10401; *Small* 2006, 2(10), 1134-1138; *Analytical Chemistry* 2006, 78(19), 6974-6979; 2007, 79(20), 7644-7653; 2008, 80(22), 8477-8484; 2009, 81(22), 9314-9320; 2010, 82(16), 7008-7014; 2011, 83(7), 2685-2690; 2012, 84(3), 1380-1385) and several patents.

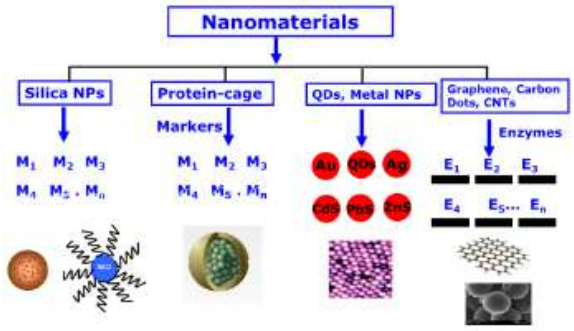

Figure 5 Biofunctionalization of nanomaterials for bioassays, bioimaging, and drug delivery.

6. Single-atom catalysts for fuel cells and water splitting applications

Recent years have witnessed a dramatic increase in the production of sustainable and renewable energy. Of particular interest are the studies on single-atom catalysts (SACs), which have sparked new interests in electrocatalysis because of their high catalytic activity, stability, selectivity, and 100 % atom utilization. In this topic, Dr. Lin's group focused on the synthesis of porous M-N-C single-atom electrocatalysts and exploration of their oxygen reduction performance. By Taking advantage of the porous nanostructure and unique single-atom catalysis feature, multiscale tuning of M-N-C catalysts regarding increasing the number of active sites and boosting the intrinsic activity of each active site was realized simultaneously at a single atom scale. The obtained nanomaterials including metal-organic frameworks derived porous SACs (*Small* 2018, 14, 1703118), Fe-N-doped carbon nanotube aerogels (*Small* 2017, 13, 1603407.) and hierarchically porous M–N–C (M = Co and Fe) SACs (*Advanced Energy Materials* 2018, 8 (29), 1801956.) all exhibited excellent oxygen reduction performances. Besides, the exploration of SACs in water

splitting was also presented (*ACS Energy Letters* 2018, 3, 17 13-1721).

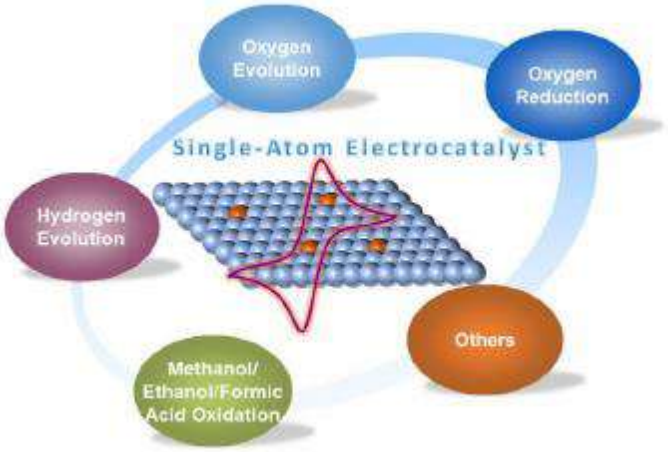

Figure 6 Single atom electrocatalysts.

Using Remotely Sensed Spatiotemporal Information to tackle Emerging Environmental Problems

by Soe W. Myint, Member EUAS

Short Biography

Education

1. *Ph.D., Geography (GIScience), Louisiana State University*
2. *M.S., Natural Resources Program (Environmental Remote Sensing and Geoinformation for Development), Asian Institute of Technology*
3. *Post-Grad. Diploma, Forest Survey (Aerospace Remote Sensing Techniques), International Institute for Aerospace Survey and Earth Sciences (ITC), the Netherlands*
4. *B.S., Forestry, Rangoon University*

Appointments

2013 – present: Professor, School of Geographical Sciences and Urban Planning, ASU
2008 – 2013: Associate Professor, School of Geographical Sciences and Urban Planning, ASU
2006 – 2008: Assistant Professor, School of Geographical Sciences, ASU
2001 – 2005: Assistant Professor, Department of Geography, University of Oklahoma
1994 – 1998: Research Specialist, United Nations Environment Program (UNEP/EAP-AP)
1983 – 1992: Dy Manager, National Forest Management/Inventory project, (UNDP/FAO/MYA/85/003)

Awards and Honors

1. *Invited to give a graduation speech at the 129th Asian Institute of Technology (AIT) Graduation Ceremony on May 18, 2018 - https://www.youtube.com/watch?v=-un1liwqPRo.*
2. *Member, European Union Academy of Sciences (EUAS), elected 2018.*
3. *Outstanding Paper in Landscape Ecology, 2017 (Co-author). United States International Association for Landscape Ecology, US-IALE annual meeting, Baltimore.*
4. *Outstanding Achievement Award – American Association of Geographers (AAG) - Remote Sensing Specialty Group (RSSG), 2016 AAG Annual Meeting, San Francisco. According to AAG-RSSG, this Award is the most prestigious award for established remote sensing scholars at AAG.*
5. *Prominent Alumnus of AIT - Received the title of Prominent Alumnus of Asian Institute of Technology (AIT), http://www.aitalumni.com/prominent-alumni-people.*
6. *2015 Best Imported Book Award given by the China Press Association – Chinese version of the book titled "Advances in Mapping from Aerospace Imagery: Techniques and Applications" My chapter contribution: Myint, S.W., 2012. The effects of the spatial pattern of vegetation cover on urban warming in a desert city, Taylor and Francis Group, LLC, pp 261-278.*
7. *Success Story - Among those awarded as Prominent Alumni, my biography was published under 'Success Stories' of the Asian Institute of Technology (AIT) Alumni Association, http://www.aitalumni.com/success-stories-view/10.*
8. *Nominated for the Zebulon Pearce Distinguished Teaching Award (given to tenured and tenure-track faculty members), 2017.*
9. *Honored Guest (2009) College of Liberal Arts and Sciences Convocation ceremony, for making difference in multiple undergraduate students' education, Arizona State University.*
10. *ASPRS Conference Management Award (2010) Recipient. Received at the 2010 American Society for Photogrammetry and Remote Sensing (ASPRS) annual conference in San Diego (April 26-30, 2010).*
11. *AITAA Distinguished Alumni Award (2007) for Academic and Research Excellence, Asian Institute of Technology.*
12. *Best Paper Award for Early Career Scholars in Remote Sensing, Remote Sensing Specialty Group - AAG, 2007 - Published in PE&RS journal.*
13. *CPGIS Scholar, 2005, selected by the Chinese Professionals in Geographic Information Science Abroad (CPGIS) to give lectures and research presentations at Jiangxi Normal University, Nanchang University, and Hubei University as part of the CPGIS Young Scholar Summit.*
14. *CSISS Scholarship (Center for Spatially Integrated Social Science) to attend 2003 Geographically Weighted Regression workshop, University of California, Santa Barbara.*
15. *Intergraph Young Scholar Award (UCGIS), 2002 UCGIS Summer Assembly, University of Georgia, Athens.*
16. *USGS Scholar Award, First International Conference on GIScience, 2000, Savannah, GA, USA.*
17. *Consultant (GIS) to World Health Organization (WHO), Geneva, 1999 (while studying as a Ph.D. student).*
18. *Best Student Paper Award – AAG - Remote Sensing Specialty Group, 2001 AAG meeting.*
19. *Best Student Paper Award – American Society for Photogrammetry and Remote Sensing (ASPRS) – Mid-South Region Meeting at Clemson University, South Carolina, 2000.*

20. *Best Student Paper Award (UCGIS-2000), 2000 UCGIS Summer Assembly, Portland, Oregon. 42 GIS/RS Graduate students from different Disciplines and Universities across the United States participated.*
21. *Best Poster Presentation Award, 1998 - 18th Asian Conference on Remote Sensing, Kuala Lumpur.*
22. *AAG Otis Paul Starkey Dissertation Research Award. Association of American Geographers, 2001.*
23. *William G. Haag Award (2001). Most outstanding paper in professional meetings, Dept. of Geography & Anthropology, LSU.*
24. *Best Student Paper Award (2nd place), 2000 South Western Division AAG meeting, Texas A&M University.*
25. *Best Student Paper Award (2nd place), 1999 South Western Division AAG meeting at Texas State University, San Marcos.*
26. *Robert C. West Field Research Award (Nov. 2000). Department of Geography and Anthropology, LSU.*
27. *Student Oral Paper Presentation Award and Travel Award, UCGIS-2000. UCGIS Summer Assembly, Portland, Oregon.*
28. *Scholars Enhanced Assistantship Award and Tuition Award (Graduate School), LSU (1999 - 2001).*
29. *Graduate School Travel Awards (3 awards): Graduate School, Louisiana State University [(October, 1999), (April, 2000), (October, 2000)].*
30. *Best Student Award, 87th Public Service Officers Training Course (No. 87), Public Service Selection and Training Board, Myanmar, 1987.*
31. *Best Student Award, Basic Officer Training Course No.1 – Myanmar Timber Enterprise, Ministry of Forestry, Myanmar, 1986.*
32. *Netherlands Government's Fellowship, Post Grad Diploma studies at ITC, the Netherlands (1988 - 1989).*
33. *French Government Scholarship, M.S. - Asian Institute of Technology, Bangkok (1993 - 1994).*

His *research* focuses on deforestation, landscape modeling, simulation and growth prediction, urban climate change, land degradation, ecosystem services, water use, carbon release, atmospheric emission, climate adaptation, drought, land use land cover change, human-environment interactions, socio-economic analysis, variation, and extreme, urban heat island, climate adaptation, human-environment interactions, surface and ground water changes, crop water use, flood simulation, urban image classification, urban spatial modeling, risk analysis, mitigation, recovery, and monitoring, uncertainty, urban emission, land fragmentation, evapotranspiration modeling, land fragmentation, regional climate change modeling, urban water use, urban growth prediction, local scale urban meteorological parameterization, urban heat island, degradation of ecosystem, carbon flux, aerosol assessment, disaster assessment, algorithm development, data mining, GIScience, spatial statistics, spatio-temporal analysis, and spatial model development.

Our planet has been experiencing significant changes in global population, urbanization, energy use, food security, water use, climate, and atmospheric conditions since the last few decades. These changes are emerging along with the rapid growth of data and advanced analysis approaches. The integrative space-time system of geographic information science offers a unique and effective framework to investigate spatio-temporal processes and interactions in a wide range of environmental applications for informed decision-making. Soe Myint has demonstrated if and how spatial-temporal image analysis can be employed to tackle some emerging environmental issues in connection to evidence-based sustainable decision making. Example applications and their respective findings are given below.

(1) Estoque, R.C., S.W. Myint, C. Wang, A. Ishtiaque, T.T. Aung, L. Emerton, M. Ooba, H. Yasuaki, M.S. Mon, Z. Wang, C. Fan, 2018, Assessing environmental impacts and change in Myanmar's mangrove ecosystem service value due to deforestation (2000-2014), Global Change Biology, DOI: 10.1111/gcb.14409.

In this study, we quantified Myanmar's mangrove forest cover changes between 2000 and 2014 using remotely sensed data, examined the environmental impacts of such changes, and estimated the changes in the economic values of mangrove ecosystem services in the country. Results indicate that Myanmar had a net mangrove loss of 191,122 ha over the study period. Since 2000, Myanmar has been losing mangrove forest cover at

an alarming rate of 14,619 ha/year (2.2%/year). The observed mangrove forest cover loss has resulted in decreased evapotranspiration, carbon stock, and tree cover percentage. Due to deforestation, Myanmar also suffered a net loss of 2,397 million US$/year in its mangrove ecosystem service value (i.e. 28.7% decrease from 2000), in which maintenance of fisheries nursery populations and habitat and coastal protection were among those services that were greatly affected. We suggest that intensive reforestation and mangrove protection programs be implemented immediately. Agroforestry and community forestry programs are encouraged in areas that are under immense pressure from paddy field expansion, fuelwood extraction, charcoal production, and fish and shrimp farming activities.

(2) Ishtiaque, A., S.W. Myint, C. Wang, 2016. Examining the ecosystem health and sustainability of the world's largest mangrove forest using multi-temporal MODIS products, Science of the total Environment, 569-570: 1241-1254. http://www.sciencedirect.com/science/article/pii/S0048969716313870.

Sweeping across Bangladesh and India, the Sundarbans forest is the world's largest contiguous mangrove forest. In this paper, we used MODIS land products to compare the spatiotemporal ecological dynamics of the Bangladesh and Indian part of this mangrove forest between 2000 and 2010.Weused the following 5 ecological parameters for our analysis: the Percent Tree Cover (PTC), Enhanced Vegetation Index (EVI), Net Primary Productivity (NPP), Leaf Area Index (LAI), and Evapotranspiration (ET). Our pixel-based time-series trend analysis for each MODIS image stack, using an ordinary least square (OLS) regression method, showed that forest degradation is happening in fragmented parcels within the forest. The degradation rate is comparatively higher in the Bangladesh part than in the Indian part of Sundarbans. Compartments 8, 10, 12, and 15 in the Bangladesh part, in particular, show high degradation, while compartment 48 and the southern edge of 45 shows light increases in PTC or EVI. Forest degradation in the Indian part of the forest is evident in the National Park and Reserve Forest blocks; however, no substantial degradation is evident in the western section. We have identified certain anthropogenic stressors (i.e., oil pollution, shrimp farming) and natural stressors (i.e., increased salinity, cyclones, forest fire) which might be responsible for the observed degradation. We have provided sustainable planning options and policy transformation alternatives for those areas under pressure from these stressors.

(3) Fan, C., S.W. Myint, S. Rey, and W. Li, 2017. Time series evaluation of landscape dynamics using annual Landsat imagery and spatial statistical modeling: Evidence from the Phoenix metropolitan region, International Journal of Applied Earth Observation and Geoinformation, 58:12-25.

In this paper, we integrate annual image time series, continuous spatial indices, and non-parametric trend analysis into a spatiotemporal study of landscape dynamics over the Phoenix metropolitan area from 1991 to 2010. We harness local indicators of spatial dependence and modified Mann-Kendall test to describe the monotonic trends in the quantity and spatial arrangement of two important land use land cover types: vegetation and built-up areas. Results suggest that declines in vegetation and increases in built-up areas are the two prevalent types of changes across the region. Vegetation increases mostly occur at the outskirts where new residential areas are developed from natural desert. A

sizable proportion of vegetation declines and built-up increases are seen in the central and southeast part. Extensive land conversion from agricultural fields into urban land use is one important driver of vegetation declines. The xeriscaping practice also contributes to part of vegetation loss and an increasingly heterogeneous landscape. The quantitative framework proposed in this study provides a path way to effective landscape mapping and change monitoring from a spatial statistical perspective.

(4) Wang, C., S.W. Myint, P. Fan, M. Stuhlmacher, and J. Yang, 2018. The Impact of Urban Expansion on the Regional Environment in Myanmar: A Case Study of Two Capital Cities, Landscape Ecology, 33(5):765-782.

This study examines the spatio-temporal patterns of urban expansion for Yangon and Nay Pyi Taw, the former and new national capitals of Myanmar, and its impact on the regional environment between 2000 and 2013. The objective is to examine different driving forces of urban expansion for Yangon and Nay Pyi Taw, and their environmental consequences during Myanmar's transitional economy. Classified time-series Landsat images are used to evaluate urban expansion processes. A time-series trend analysis technique is used to examine the environmental consequences. The built-up areas in Nay Pyi Taw and Yangon exhibit exponential and polynomial increase, respectively. A 1% increase of built-up area could potentially cause an increase of daytime LST of 0.7 _C, a PTC loss of 2.3%, a decrease in NPP of 34.3 kg/m2, and an ET decrease of 42.2 mm for Yangon. Similarly, for Nay Pyi Taw, a 1% increase in built-up area could potentially cause a daytime LST increase of 0.3 _C, a nighttime LST increase of 0.06 _C, a PTC loss of 2.5%, a decrease in NPP of 15.1 kg/m2, and a decrease of 19.2 mm ET. No significant change was observed for AOD for either city. Both cities have experienced extensive urban expansion but with different spatial and temporal characteristics, and their effects on the regional environment are different.

(5) Wang, C, Wang, C., S.W. Myint, and Z. Wang, 2017. Landscape determinants of spatio-temporal patterns of aerosol optical depth in the two most polluted metropolitans in the United States, Science of the Total Environment, 609(2017):1556–1565.

Elevated concentration of atmospheric aerosols during severe urban air pollution episodes necessitates a deep understanding of the underlying determinants for a sustainable urban environment. The 15-year (2001–2015) Moderate Resolution Imaging Spectro-radiometer (MODIS) aerosol optical depth (AOD) data for the Phoenix and Los Angeles Metropolitan Areas were applied to examine the spatio-temporal patterns and dynamics of urban aerosols. The strongly correlated temporal trends of AOD were observed due to the similar seasonal pattern of aerosol emissions and potential synoptic connections between two areas. Relatively higher mean value and lower decreasing trend of AOD were found in the PMA. Correlations reveal that topography is the predominant factor affecting the spatial pattern of AOD, as compared to the urban land use and vegetation. The effect of urbanization on air pollution varies with preexisting landscape, which apparently alleviates aerosol concentration in the PMA. Vegetation mitigates air pollution despite its emission of fine mode aerosols. As a cross-validation, the ground-measured concentrations of particulate matters ($PM_{2.5}$ and PM_{10}) were compared against AOD. The abnormal weak positive or strong negative AOD-$PM_{2.5}$ associations result from the relatively small portion of anthropogenic aerosols and the changing atmospheric boundary layer height.

Novel Nanoscience in Superfluid Helium

by Shengfu Yang, Member EUAS

Short Biography

Professor in Physical Chemistry and NanoChemistry, Department of Chemistry, University of Leicester – Leicester

Prof. Shengfu Yang is currently a Professor in Physical Chemistry and NanoChemistry. He graduated BSc in Applied Physics from Department of Physics, Tsinghua University in 1992, followed by MSc studies in Physical Chemistry at Dalian Institute of Chemical Physics and PhD studies in Physical Chemistry at University of Science and Technology of China, where he obtained his MSc and PhD degrees in 1995 and 1997, respectively. He then started to work in several world-class laboratories at Université Joseph Fourier de Grenoble, Massachusetts Institute of Technology, University of Helsinki and University of Leicester, where he had been involved in several research programmes and has acquired a wide range of experience in physical chemistry and nanoscience. At Leicester, he was awarded a highly prestigious EPSRC Advanced Research Fellowship in 2006, before being appointed to a senior lectureship in 2011 and a readership in 2014. In each stage of his research career he has led new research programme involving development of cutting-edge technologies; hence his expertise covers molecular spectroscopy, laser techniques, electro-optical systems, computational chemistry, mass spectrometry, helium nanodroplets, and nanoscience. In recognition of his outstanding and pioneering research in developing novel nanoscience in superfluid helium droplets, he received the Merit Award at the University of Leicester in 2012, and a Nanoscience Award by Cognizure in 2015.

Prof. Yang has established an international leadership in both Physical Chemistry and Nanoscience based on superfluid helium droplets. He has made several important discoveries on physical chemistry and fundamental of superfluid helium and has pioneered novel nanoscience using superfluid helium droplets as the growing medium. He invented several key techniques that can significantly broaden the landscape of superfluid helium in nanoscience, such as seeding technique, optical-selection technique, new techniques for the formation of high-moment magnetic nanoparticles and core-shell metal-semiconductor nanowires. These can have profound impact on biomedical diagnostics and treatment, data storage, quantum information transportation, sensing technology and the energy industry. Currently, he is leading several interwoven research programmes, including 1) spectroscopy of molecules and clusters, 2) single-atom catalysed reactions, 3) direct growth of nanoparticle assemblies using molecular templates, 4) high-moment magnetic nanoparticles beyond the bulk limits and 5) photonic nanoparticles and nanowires. His research has attracted over £2M of external grants from the EPSRC and the Leverhulme Trust as the principal investigator.

Prof. Yang is well connected with the science community of physical chemistry as evidenced by numerous invitations to work with various learned societies and editorial boards. He is a committee member of the Spectroscopy and Dynamics Group (SDG) of the Royal Society of Chemistry, and the Chinese Society of Chemical Science and Technology in the UK (CSCST-UK). In addition, he is a Fellow of Royal Society of Chemistry, a member of the EPSRC Peer Review College, an associate editor for Nano-micro Letters, a member of the editorial board for Physical

Chemistry, Journal of Molecular & Analytical Techniques, and a referee for a number of scientific journals. He is also a distinguished professor in several Chinese universities.

The selected articles highlight the key milestones towards establishing superfluid helium droplets as a tool for novel nanoscience.

1. **Jun Liu, Ben Shepperson, Andrew Ellis and Shengfu Yang, "Core-shell effects in the ionization of doped helium nanodroplets", *Phys. Chem. Chem. Phys*. 13, 13920-13925 (2011).**

Core–shell particles with water clusters as the core and surrounded by an atomic or molecular shell have been synthesized for the first time by adding water and a co-dopant sequentially to helium nanodroplets. The co-dopants chosen for investigation were Ar, O_2, N_2, CO, CO_2, NO and C_6D_6. These co-dopants have been used to investigate the effect of an outer shell on the ionization of the core material by charge transfer in helium nanodroplets. The specific aim was to determine how the identity of the shell material affects the fragmentation of water cluster ions, *i.e.* whether it helps to stabilize parent ion ($(H_2O)_n^+$) formation or increases fragmentation (to form $(H_2O)_nH^+$). N_2, O_2, CO_2 and C_6D_6 all show a marked softening effect, which is consistent with the formation of a protective shell around the water cluster core. For CO and NO co-dopants, the response is complicated by secondary reactions which actually favour water cluster ion fragmentation for some water cluster sizes.

2. **Adrian Boatwright, Cheng Feng, Daniel Spence, Elspeth Latimer, Chris Binns, Andrew M. Ellis and Shengfu Yang, "*Helium droplets: a new route to nanoparticles*", *Faraday Disc*. 162, 113-124 (2013).**

Helium droplets are large helium clusters that are capable of picking up individual atoms and molecules and show promise as nano-reactors for the synthesis of unique nanoparticles. In particular, the sequential addition of materials of different types offers opportunities for the fabrication of novel core–shell nanoparticles that cannot be synthesised by other methods. To exploit this potential, here we have carried out a mass spectrometry investigation on metal clusters in order to establish how to control the doping conditions for the fabrication of nanoparticles in superfluid helium droplets, and in particular to develop a recipe to control core and shell ratios in the case of core–shell nanoparticles. Several types of metal nanoparticles, including pure Ag, Au and Ni nanoparticles, and Ag/Au and Ni/Au core–shell systems, have been synthesised and then removed from the helium droplets by deposition on substrates for *ex situ*investigations using high-resolution transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). The TEM imaging has been used to estimate the sizes of nanoparticles, which show a bi-model distribution under the conditions employed. We also present the first evidence that crystalline metal nanoparticles are formed by self-assembly of metal atoms in helium droplets. The XPS investigation of Ni/Au core–shell nanoparticles shows an absence of any Au 4f core-level shift that would occur on alloying of Au and Ni, which provides the first direct evidence for the successful formation of core–shell nanoparticles using superfluid helium droplets.

3. **Daniel Spence, Elspeth Latimer, Cheng Feng, Adrian Boatwright, Andrew M. Ellis and Shengfu Yang, "*Vortex-induced aggregation in superfluid helium droplets*", *Phys. Chem. Chem. Phys*. 16, 6903-6906 (2014).**

The formation of Ag nanoparticles by the addition of Ag atoms to helium droplets has been investigated. The resulting nanoparticles were then imaged by transmission electron microscopy after being deposited on a thin solid surface. In large helium droplets chains of Ag nanorods were observed similar to recently reported track-like deposits [Gomez *et al.*, *Phys. Rev. Lett.*, 2012, 108, 155302]. However, by adjusting the experimental conditions chains of spherical nanoparticles could also be seen with a nearly uniform inter-particle spacing. Given that spherical Ag nanoparticles have no intrinsic anisotropy, the only viable explanation is that these particles must be guided into position by interaction with a quantized vortex spanning the diameter of the helium droplet. Furthermore, addition of Si to the droplets immediately after Ag resulted in Si inserting between the Ag nanoparticles to form continuous nanowires. This eliminates the possibility that the segmented Ag nanostructures are the result of nanowire fragmentation when the helium droplets collide with the deposition substrate. Thus segmented Ag chains are shown to be an intrinsic feature of Ag aggregation in helium droplets in the presence of a quantized vortex.

4. **Elspeth Latimer, Daniel Spence, Cheng Feng, Adrian Boatwright, Andrew M. Ellis and Shengfu Yang, "*Preparation of ultrathin nanowires using superfluid helium droplets*", *Nano Lett.* 14, 2902-2906 (2014).**

Direct preparation of long one-dimensional (1D) nanostructures with diameters <10 nm inside superfluid helium droplets is reported. Unlike conventional chemical synthetic techniques, where stabilizers, templates, or external fields are often required to induce 1D growth, here, we exploit the use of quantized vortices to guide the formation of ultrathin nanowires. A variety of elements have been added to the droplets to demonstrate that this is a general phenomenon, including Ni, Cr, Au, and Si. Control of the length and diameter of the nanowires is also demonstrated.

5. **Shengfu Yang, Cheng Feng, Daniel Spence, Aula M. A. A. Al Hindawi, Elspeth Latimer, Andrew M. Ellis, Chris Binns, Davide Peddis, Sarnjeet S. Dhesi, Liying Zhang, Yafei Zhang, Kalliopi N. Trohidou, Marianna Vasilakaki, Nikolaos Ntallis, Ian MacLaren, and Frank M. F. de Groot, "*Robust ferromagnetism of chromium nanoparticles formed in superfluid helium", Adv. Mater*. 29, 1604277 (2017).**

Chromium nanoparticles are formed using superfluid helium droplets as the nanoreactors, which are strongly ferromagnetic. The transition from anti-ferromagnetism to ferromagnetism is attributed to atomic-scale disorder in chromium nanoparticles, leading to abundant unbalanced surface spins. Theoretical modelling confirms a frustrated aggregation process in superfluid helium due to the antiferromagnetic nature of chromium.

6. **Shengfu Yang, Cheng Feng, Daniel Spence, Elspeth Latimer, Andrew M. Ellis,**

A. Al Hindawi, Adrian Boatwright, Chris Binns, Davide Peddis, Kalliopi N. Trouhidou, Nikolaos Ntallis, Marianna Vasilakaki, Liying Zhang, Yafei Zhang and Sarnjeet S. Dhesi, "*Ferromagnetic nanoparticles with magnetic moments far exceeding the bulk limit*". *PNAS* (under review).

The production of ever more powerful nanomagnets holds promise in numerous areas of science and technology. By growing nanoparticles atom-by-atom in very cold superfluid helium droplets, we obtained the largest enhancement of the magnetic moment in a ferromagnetic nanoparticle (nickel) relative to the bulk value yet seen and the preservation of this moment on exposure to air by a protective shell. The magnetic moment of the nickel contents in Ni/Au and Ni/Ag core-shell nanoparticles was found to be over 2 μ_B/atom at 300 K, which is more than 3 times larger than the bulk limit of nickel. At 5 K the magnetic moment reached 4.26 μ_B/atom, approaching the single atom limit of nickel. We propose that superfluid helium suppresses the thermal effect by continuous rapid cooling and thus accentuates the effect of exchange interactions during the atom-by-atom growth of nickel nanoparticles. This results in a new high-spin structure in nickel nanoparticles, which is supported by both TEM imaging and theoretical modelling.

Research Activities of Prof Gleiter at the Institute of Nanotechnology (INT) of the Karlsruhe Institute of Technology (KIT)

by Herbert Gleiter, Member EUAS

Short Biography

Professional Career

Since 2015 ***Senior Fellow*** *(jointly with the Nobel and Fields Medal Laureates Haroche, Lehn and Small) of the Institute of Advanced Studies,* ***City University of Hong Kong.***

Since 2012 ***Founding Director*** *of the* ***Herbert Gleiter Institute of Nanoscience*** *of* ***Nanjing University*** *of Science and Technology, Nanjing, P.R.China*

Since 2006 ***Institute Professor*** *and* ***Distinguished Fellow*** *of the* ***Institute of Nanotechnology****, Karlsruhe Institute of Technology (KIT), Germany*

2007 - 2010 ***Distinguished Professor, Arizona State University****, Phoenix, USA*

2005 ***Distinguished Scholar*** *of the* ***Korean Research Foundation,*** *Seoul, Korea*

2004 - 2007 ***Kuang-pui Chair Professor, Zhejiang University****, Hangzhou, PR China*

1998 - 2004 ***Director*** *of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

1998 ***Founding Director*** *(jointly with Profs. J M Lehn and D. Fenske) of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

1994 - 1998 ***Member*** *of the* ***Executive Board*** *of the* ***Research Center Karlsruhe****, Germany*

1987 - 1994 ***Founding Director*** *of the* ***Institute*** *of* ***New Materials****, Saarbruecken, Germany*

1982 *Call to the* ***Federal Institute of Technology (ETH****) Zurich, Switzerland*

1980 *Call to the* ***University of Hamburg****-Harburg, Germany*

1973 -1994 ***Professor/Director*** *of the* ***Institute*** *of* ***Material Science****, University of the Saarland, Germany*

1972 ***Professo****r, Institute of Materials Science,* ***University Bochum****, Germany*

1971 ***Visiting Scientist*** *of the* ***Massachusetts Institute of Technology (MIT),*** *Cambridge, USA*

1970 *D. Sc. (Habilitation)* ***in Material Science*** *at the University of Bochum, Germany*

1966 - 1969 ***Research Fellow*** *at* ***Harvard University*** *Cambridge, USA*

1966 *Ph.D. in* ***Physics*** *at the Technical University of Stuttgart, Germany*

1959-1965 *Student of* ***Mechanical Engineering and Physics*** *at the Technical University of Stuttgart*

Honours and Awards (selection)

2018 ***Jan Czochralski Medal and Award,*** *Polish Academy of Science, Warsaw University,*

2016 ***Friendship Award*** *and* ***Medal of Merit*** *of Chinese Government, Jianzu, China*

2015 ***Cothenius Medal*** *of the German National Academy of Sciences - Leopoldina*

2015 ***Honorary Doctor*** *of the City University of Hong Kong*

2014 ***2014 Distinguished Lecturer****, University of Hong Kong*

2012 ***Zijin Chair Professor Award*** *of the Herbert Gleiter Institute of Nanoscience of the Nanjing University of Science and Technology, Nanjing, China*

2012 ***Nanomaterials Award 2012***

2012 ***Edward DeMille Campbell Award****, American Society for Metals (ASM)*

2009 ***R.F. Mehl Award*** *of the Minerals, Metals, Materials Society, USA*

2009 ***Blaise Pascal Medal*** *of the European Academy of Sciences, Belgium*

2009 ***NANO Today Award*** *of the Agency for Science, Technology Research, Singapore*

2008 ***Honorary Doctor*** *of the University of Muenster, Germany*

2008 ***Honorary Doctor*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

2008 ***Achievement Award NANOSPD*** *Int. Steering Committee*

2008 ***Staudinger-Durrer Award*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

2008 ***Honorary Member*** *of the German Materials Society DGM*

2008 ***Von Hippel Award*** *of the Materials Research Society, USA*

2007 ***Gold Medal*** *of Acta Materialia*

2006 ***Humboldt Medal*** *of the Alexander von Humboldt Foundation, Germany*

2005 ***Distinguished Scholar*** *of the Korean Research Foundation*

2004 ***Honorary Professor*** *of Lanzhou University, PR China*
2004 ***H. Lee Lecture Award*** *of Chinese Academy of Science*
2004 ***Honorary Professor*** *at Zhejiang University, Hangzhou, PR China*
2003 ***Nanomaterials Award*** *of the Deutsche Bank, Germany*
2002 ***Honorary Doctor*** *of the Technical University of Darmstadt, Germany*
2000 ***Van Horn Award*** *of Case Western University Cleveland, USA*
1999 ***Werner Heisenberg Medal*** *of the Alexander von Humboldt Foundation, Germany*
1998 ***Heyn Medal*** *of the German Society for Materials Science*
1995 ***Gold Medal*** *of the Federation of European Material Societies (FEMS), Belgium*
1993 ***Vinci of Excellence Award*** *of the Hennessy-Vuitton Foundation, France*
1993 ***Max-Planck-Research Prize*** *of the Humboldt Foundation and the Max Planck-Society, Germany*
1992 ***Member of the President's Council*** *of the University of Illinois, USA*
1992 ***TMS Lecture Award*** *of the US Minerals, Metals and Materials Society*
1991 ***Order of Merit*** *of Saarland, Germany*
1988 ***Leibniz Prize*** *of the German National Science Foundation (DFG)*
1984 ***Alcoa Prize*** *of the Alcoa Foundation, USA*
1979 ***Karl-Schurz Award*** *of the University of Wisconsin, USA*
1972 ***Masing Prize*** *of the German Society for Metals*

Memberships in National Academies

1998 Member of the ***German National Academy of Sciences*** *– Leopoldia, Germany,*
2004 Member of the ***US National Academy of Engineering***
2004 Member of the ***American Academy of Arts and Sciences***
2006 Member of the ***Indian National Academy of Engineering***
2007-12 ***Vice President*** *of the* ***German National Academy*** *of Sciences*
2009 Member of the ***European Academy of Sciences***
2009 Member of the ***Indian Academy of Sciences***
2011 Member of the ***Indian Science Academy***
2014 Member of the ***Academia Europaea***
2014 Member of the ***European Academy of Sciences and Arts***
2015 Member of the ***EU Academy*** *of* ***Sciences***
2016 Member of the ***US National Academy of Inventors***

Founding of a New Research Institute

*Founding of the "****Herbert Gleiter Institute of Nanoscience****" in 2012 at Nanjing University of Science and Technology. This Institute is planned to have a size and a structure of a Max Planck Institute in Germany.*

Today's technologies are based primarily on utilizing crystalline materials such as metals, semiconductors or crystalline ceramics. The reason for this preference of crystalline materials is that their properties can be varied by varying their chemical compositions (by alloying, doping) and/or by varying their microstructures by means of introducing microstructural defects such as inter-crystalline interfaces, dislocations and/or point defects. In the late 1970s the variation of the properties of crystalline materials by introducing a very high density of defects opened the way a new class of materials: nano-crystalline materials. The work of the research group at Karlsruhe headed by Herbert Gleiter made several fundamental contributions to the development of this field that were in recent years internationally recognized by the award of several international prizes such the Jan Czochralski Award of the Polish academy of Sciences and E-Mrs, the Cothenius Medal the highest recognition of the German National Academy of Sciences,

Leopoldina, the Honorary Doctorates of the City University of Hong Kong, the University of Muenster and the ETH Zuerich, the Nanomaterials Award, the Edward DeMille Campbell Award of the American Society for Metals and the R.F. Mehl Award of the Minerals, Metals, Materials Society, USA

This new concept of nanocrystalline materials confirmed after its proposal by a rapidly growing number of subsequent studies. Today more than 800 papers are published in this area every year, several international conferences are organized annually and most (national as well as international) conferences in the area of Materials Science have one or several sessions on "nano-materials".

About 10 years ago the studies of Prof Gleiter's group opened the way to a new world of technologies based on non-crystalline materials may be opened by means of nano-glasses. Nano-glasses consist of nanometer-sized glassy regions connected by (nanometer-wide) interfacial regions with atomic and electronic structures that do not exist in melt-cooled glasses. If the size of the nanometer-sized glassy regions is 5 nm or less, the volume fraction of these interfacial regions is 50% or above. Due to their new atomic/electronic structures, the properties of nano-glass differ from the corresponding properties of melt-cooled glasses. For example, FeSc nano-glasses were (at 300K) strong ferro-magnets although the corresponding melt-cooled glasses were paramagnetic.

Similarly, the ductility, the biocompatibility, the catalytic properties of nano-glasses were improved by up to several orders of magnitude. Moreover, nano-glasses open the way to new kinds of alloys as they permit the alloying of components that are immiscible in crystalline materials. This applies to components with the same as well as different kinds of chemical bonds. Nanoglass alloys of Fe90Sc10 and Cu64Sc36 glasses are an example of two metallic components (Cu and Fe) that are immiscible in the crystalline state. Alloys of metallic Fe90Sc10 glasses and SiO2 glasses are nano-glass alloys of the second type.

Just like in the case of nano-crystalline materials, the properties of which may be changed by varying the sizes and/or chemical compositions of the crystallites, the properties of nano-glasses may be controlled by varying the sizes and/or chemical compositions of the glassy clusters. This analogy opens the perspective that a new age of

technologies - a ”glass age”- may be initiated by utilizing the new properties of nano-glasses and modifying their properties by varying the sizes and/or chemical compositions of the glassy clusters.

The pioneering work opening the field of nano-glaasses was internationally recognized by the award of several prizes (some of which are mentioned above) and his election - during the past five years - into the following National Academies: the Indian Science Academy, the Academia Europaea, the European Academies of Sciences and Arts and EU Academy of Sciences and as a foreign member of the US National Academy of Inventors. In 2012 the University of Nanjing founded the “Herbert Gleiter Institute of Nanoscience” and appointed him as the Institute’s Founding Director.

Recognition of Proteins by the Immune System - a Model for Investigating other Protein Molecular Recognition

by M. Zouhair Atassi, Member EUAS

Short Biography

B.Sc. Special Honours in Chemistry, University of Bristol, England
M.Sc. in Chemistry, University of Birmingham, England
Ph.D. in Chemistry, University of Birmingham, England
DSc. in Chemistry, University of Birmingham, England

Positions

July 1, 2017- Present *Emeritus Robert A Welch Chair of Chemistry, Em. Professor of Biochemistry and Molecular Biology. Em. Professor of Pathology and Immunology*
Editor-in-Chief, Critical Reviews in Immunology
Editor-in Chief, Protein Reviews
1983 – 2017 *Robert A. Welch Chair of Chemistry*
Professor of Biochemistry and Molecular Biology
Professor of Pathology and Immunology
Baylor College of Medicine, Houston, Texas 77030, USA
1975 – 1983 *Professor of Biochemistry and Professor of Immunology*
Mayo Medical School, Rochester, Minnesota
Also, Professor of Biochemistry and Professor of Immunology,
University of Minnesota, Minneapolis, Minnesota
1971 – .1975 *Professor and Chairman, Biochemistry Division*
Wayne State University, Detroit, Michigan
1968 – 1975 *Professor of Chemistry*
Wayne State University, Detroit, Michigan
1963 – 1968 *Assistant Professor of Biochemistry*
State University of New York at Buffalo, Buffalo, New York.
1962 – 1963 *Postdoctoral Research Fellow*
Division of Laboratories and Research, New York State Health Department, Albany, NY.
1960 – 1962 *Postdoctoral Research Fellow in Chemistry*
University of Birmingham, Birmingham, England

Recognition

For my findings that immune responses target specific sites on a protein surface, I received many honors and awards. Among them the degree of DSc from the University of Birmingham, UK (1973); the Kuwait Prize in Basic Sciences (1994); the Harden Medal and Jubilee Lecture of the Biochemical Society, London (1987). The Biochemical Society states the (Jubilee) "lecturer . . . will be a biochemist of distinction from any part of the world". (2004) NASA Space Act Award in recognition for inventions and other scientific and technical contributions. (1996) The Japanese Society of Electrophoresis Award for Outstanding Research Contributions; 1988 Tohuku Medical Society Award For pioneering research contributions; In 1979, I was named Distinguished Lecturer in Medical Science at Mayo Medical School, and have since been named Distinguished Lecturer or honorary professor by over 10 US universities and foreign institutions.
My scientific contributions have received considerable attention in science news sections and editorials, both in the US and in Europe. The impact on biology and medicine of my myoglobin work was depicted as an "immunological tour de force" by Scientific American (March, 1976) and was hailed as worthy of the Nobel Prize by Niewsblad van het Noorden of the Netherlands (July, 1976). My achievements were featured by Nature and Science in their research news. Other aspects of my work were described in various other lay and scientific publications such as the Guardian in Britain (March, 1980) and Clinical Chemistry News in the United States (January, 1981). The impact of my acetylcholine receptor breakthroughs on central nervous system drug design was featured by an editorial in the Journal of NIH Research (December 1990).
I have published over 500 research articles and edited/co-edited 34 books. I have held, and currently hold, many important scientific positions: Editor-in-Chief, Critical Reviews in Immunology, and Protein Reviews; Chair, Editorial Committee of Immunological Investigations; Editor-in-Chief: J. Protein Chemistry (1978-2004, The Protein Journal (2004-2017); Editorial Board member of a number of other journals; member Advisory Board of the Neurotoxin Institute; member of the Scientific Advisory Board of Center for Bio-security Science, Los Alamos National Laboratory; President of the Institute of Immunobiology and International Symposium of Immunobiology, member of the Selection Committees of King

Faisal International Prize for Science and for Medicine. Previous positions include: Member of the Edman Award Selection Committee, Chairman of the 1994 International Conference on Methods in Protein Structure Analysis (MPSA), co-chair of International Conference of Neurotoxins (ICON 2006).

Abstract

I was the first to map the complete antigenic structures of proteins. After over 10 years of intensive research, I completed mapping of myoglobin (1) (in 1975), and after 12 years lysozyme (in 1978) (2). These were the first two proteins for which immune recognition of the molecules were determined precisely. The accomplishments were followed by the detailed mapping of the antigenic sites of over12 more proteins (allergens, α-neurotoxins, influenza A hemagglutinin, botulinum neurotoxins A and B, and the autodeterminants of acetylcholine receptor, human chorionic gonadotropin, thyrotropin receptor, insulin receptor) as well as the sites recognized by T-cells. The studies showed that the antibody (Ab) and T cell recognition sites are controlled separately by the major histocompatibility complex (MHC) of the host, and by T- and B-cell epitope interactions. Autoimmune and allergic responses are under genetic control and could be lowered by tolerogen-peptide or by Abs against the epitope-binding region on associated MHC of the host. These contributions opened up new vistas for molecular immunology and provided strategies for molecular, clinical and therapeutic benefits.

Overview

In the 1960s and early 70s, the mechanisms underlying immune recognition of proteins were poorly understood. It was believed that a protein is recognized by antibodies (Abs) as a whole, yet Abs and T cells were thought to target different features. It was unknown how T- and B- cells interacted or how the responses were controlled. Peptides were thought to become immunogenic only by coupling "haptenization" to a carrier. In the late 60s myoglobin and lysosyme were the only proteins for which the primary and 3-dimensional structures were known. In 1975 and 1978, applying and devising tools of chemistry, I completed the mapping and synthesis of the antigenic sites (epitopes) of myoglobin and lysozyme, respectively. These were the first two proteins for which antigenic structures were determined. We have since determined the full antigenic structures of at least 10 more proteins and mapped their T-cell recognition. In a series of articles in 1977-1981, I was the first to provide the comparison of T- and B-cell recognition of proteins at the sub-molecular level. We demonstrated the role of epitope-specific interactions involving T- and B-cells. We also showed that Ab and T-cell responses to each epitope on a protein are controlled separately by the Major Histocompatibility Complex (MHC) of the host. These findings provided molecular and cellular bases for immune responses. Our pioneering discovery that small (6-7 residues) synthetic peptides are immunogenic provided a powerful tool in biology and medicine.

We defined and synthesized the acetylcholine receptor (AChR) functional sites, including those that bind acetylcholine, α-neurotoxins, autoAbs and/or T-cells. AChR is key for neuro-transmission at the postsynaptic neuromuscular junction. Identification of its functional sites provided molecular explanation for myasthenia gravis, an autoimmune disease to AChR. We found 2 or 3 auto-epitopes, presented by certain DQ haplotypes, were pathogenic. We devised means for manipulating autimmunity by epitope-specific immune tolerance, suppression by tolerogen-conjugated pathogenic epitopes or by Abs against peptides mimicking the rim of the epitope-binding region on the correlate HLA allele. This afforded a tool for manipulating autoimmune responses by selectively targeting epitope-binding region on the presenting MHC allele(s) without affecting immune functions of other MHC molecules. We determined and synthesized the functional regions on human DR2 antigen, a genetic restriction molecule involved in antigen presentation to human T cells. We defined the functional sites of allergens, α-bungarotoxin, and influenza A hemagglutinin. Immunization with synthetic α-bungarotoxin or influenza A virus epitopes was effective in protection against the correlate agent. Most recently, we reported the localizations of the binding sites to the receptor, and the Ab and T cell recognition sites on botulinum neurotoxins types A and B. These large protein toxins (almost 1300 residues each), are the most toxic substances known. The findings explained how the immune system defends against these toxins and paved the way for rational designs of anti-toxin synthetic vaccines. My laboratory's contributions have profoundly impacted biological sciences and provided new tools for clinical, diagnostic and therapeutic applications. I introduced powerful methodologies that are widely used for localization, molecular delineation and synthesis of a variety of protein binding sites, and regions of molecular and cellular immune responses. Most notable have been the "synthetic overlapping peptides", "surface-simulation synthesis" and small peptide immunization (introduced in 1975-1983), now widely used often without citing the discoverer. For example, a PubMed search on December 28, 2018 provided 49,663 citations for "peptide immunization".

Hemoglobin

We determined the full antigenic profiles of the alpha- and beta- chains of human hemoglobin (Hb) (3,4). Interestingly, a number of the Hb antigenic sites could be predicted by extrapolating the structural locations of myoglobin antigenic sites while the others were unique to Hb. The comprehensive synthetic strategy was also used to define the full T-cell recognition profiles of the beta- and alpha-chains. (5).

We found that the haptoglobin (Hp)-binding site on the alpha-chain of human Hb comprises residues alpha 121-127 (6**).** We also found that haptoglobin not only binds hemoglobin but also binds human myoglobin, although with an affinity that is much lower than that of hemoglobin (7). We Also, used the synthetic overlapping peptides encompassing the beta chain to localize the Hp-binding sites on the beta-chain of human Hb. (8). T cell lines and clones specific for the alpha-beta interface regions were prepared by immunization with synthetic peptides representing regions at the αβ interface of Hb. These T cells recognized the isolated correlate subunit but not the tetramer, indicating presentation without processing (9).

We employed the synthetic approach for localization of the subunit interacting surfaces in oligomeric proteins (10-12). We determined the binding activity of the uniform overlapping peptides encompassing an entire subunit to the other, radiolabeled, subunit. This permitted establishment of the full profile of peptides that bind the other intact subunit. This approach was demonstrated with human hemoglobin (10,12). Its application with the beta-chain peptides has enabled the localization of the beta-chain regions responsible for its binding to alpha-chain in solution. There was good agreement between the binding surfaces in solution and those expected from the crystal structure. There were also some significant differences in the binding levels in solution and those expected from the crystal. Peptide beta21-35 possessed much higher binding activity than would be expected from its contribution to subunit association in the crystal. Conversely, other regions expected to possess considerable binding capacity for alpha-chain either showed low (peptides beta111-125 and beta121-135) or almost no binding (peptides beta91-105 and beta101-115) capacity. On the other hand, two interacting surfaces (within peptides beta11-25 and beta71-85) that make a contribution in solution do not appear to play a role in the crystal.

We also used the overlapping peptides encompassing the alpha-chain of human hemoglobin, to map the alpha-chain regions responsible for its binding to the beta-chain in solution (10). These binding surfaces were, in general, in good agreement with those expected from the crystal structure (peptides alpha81-95, alpha101-115, alpha111-125, and alpha131-141). However, some significant differences in the binding levels were found in solution and those expected from the crystal structure. Peptide alpha31-45, which in the crystal had the highest number of contact residues of all the alpha-chain peptides, did not bind the beta-chain in solution. Similarly, peptide alpha91-105, with seven contact residues in the crystal, showed low binding with the beta-chain in solution. On the other hand, peptides alpha41-55 and alpha121-135 possessed much higher binding activity in solution than would be expected from their contribution to subunit association in the crystal. In fact, peptide alpha121-135 had the highest binding activity of the alpha-chain peptides. These studies showed that the regions of subunit association in solution are close to, but not identical with, those in the crystal.

The approach should be quite useful for mapping subunit association in oligomeric proteins and could be applied to proteins that are isolated only in traces or whose three-dimensional structure is not known.

Ra3

We also employed (13) the comprehensive synthetic approach to localize the continuous antigenic sites of ragweed allergen, Ra3. 1. We determined the full profiles of the antigenic (IgG-binding) and the allergenic (IgE-binding) sites of Ra3 and found that, the regions recognized by human IgE and by human IgG Abs coincided (14). Thus, Ra3 was found to have 4 continuous antigenic sites which occupy the same locations as the allergenic sites.

We also localized the continuous regions on Ra3 that are recognized by T cells (15) from mice immunized with Ra3. Three of the regions recognized by T cells coincided with regions recognized by Abs (i.e. B cells). But in addition to sites recognized by both T and B cells Ra3 has at least one site that is recognized exclusively by T cells and to which no detectable Ab response was detected. The findings are essential for design of anti-allergen synthetic vaccines.

Influenza hemagglutinin

We also established that protein 'continuous' antigenic sites can be localized by systematic synthetic scanning of the surface (16). The approach is useful for large complex protein molecules. Applying this approach to influenza virus hemagglutinin (HA) revealed that the antigenic structure of the hemagglutinin is more complex than had been suspected (16). We identified 12 synthetic T- and B-cell recognition regions on surface areas of the HA of X31 influenza virus. The recognition of peptides by cytotoxic T cells was MHC-

restricted (17).

The twelve X-31 peptides, in their free form, evoked anti-peptide Abs that cross-reacted with intact X31 virus. Peptides HA1-6 and HA2-10, did not induce adequate virus-specific DTH responses, but conferred 42-46% and 54-73% protection, respectively, compared to the control group that received only saline ($P < 0.03$ to $P < 0.01$). Mice were protected against lethal viral infection by synthetic peptides corresponding to B- and T-cell recognition sites of influenza A hemagglutinin.

Anti-peptides 1-11 Abs of strains A and B were bound by HA and by the intact virus of the respective strain (18). However, these antisera failed to exhibit significant virus neutralizing activity. In contrast, the monoclonal Abs that reacted with these peptides inhibited viral infectivity (19). The results clearly showed that residues 1-11 of HA2 represent an important antigenic site on influenza virus.

Antigenicity of free small synthetic peptides

We discovered, contrary to a long-held belief, that synthetic peptides of a protein, as small as six residues, when immunized in their free form (i.e., without coupling to any carrier), can elicit the formation of Abs with submolecular binding specificities to preselected protein regions (20). These peptides could represent either antigenic sites of the protein or surface regions that are not immunogenic when the intact protein is the antigen. The Abs bind specifically to the intact protein, exclusively at the region used in immunization. Monoclonal Abs with preselected specificities can also be produced from the spleens of the immunized animals (21). Free synthetic peptides have also been employed to generate T-cell lines and T-cell clones with preselected specificities to protein regions and also to induce tolerance to such preselected locations (22, 23). These breakthroughs revealed that free synthetic peptides may be used as powerful tools in basic research and in therapeutic and diagnostic applications and are demonstrated in the different sections in this concise presentation.

Effects of amino acid substitution outside antigenic site

Monoclonal Abs (mAbs) of predetermined specificity were prepared by immunizing with a free (i.e., not conjugated to any carrier) synthetic peptide representing a given antigen region of sperm whale myoglobin (SpMb). The results indicated that the reactions of mAbs, whose specificity was precisely known and predetermined by the immunizing free peptide, can be markedly affected by substitutions outside the indicated binding region on the protein.

Thus, substitutions outside an antigenic site can exert drastic effects on the binding of protein variants with mAbs whose specificity was predesigned to be against a defined site. These indirect effects and their impact on site reactivity have completely explained findings on cross-reactivities of Mb variants with mAbs of unknown specificity. They also ruled out postulations of discontinuous sites in Mb, which were based on an assumption that every substitution affecting reactivity is directly involved in binding to Ab. Results with Hb variants and mAbs of predesigned specificity gave similar conclusions.

Substitutions outside an antigenic site can exert drastic effects on the reactivity of a protein with mAbs against the site. In fact all other reports using protein mutants to localize antigenic sites are not valid. Caution should be exercised in interpreting cross-reactivity data of proteins to implicate residues as being directly in an antigenic site.

Results with Mbs and Hbs (24-26) that have no substitutions within the indicated site, clearly show that substitutions outside the site, and are not by design part of the site, can influence very markedly the reactivity of the protein variant with the anti-site mAbs. The approach can, therefore, lead to serious errors if used to identify residues of protein antigenic sites which had been postulated, on the basis of these assumptions, to constitute discontinuous antigenic sites in SpMb, were found [from the studies reported with mAbs against each of the five antigenic sites of Mb (regions 15-22, 56-62, 94-100, and 113-120 and 145-151 of SpMb)] to merely be exerting indirect effects on the observed antigenic site of Mb. The effects of substitutions, which can happen even in the absence of conformational changes, are determined by many factors, such as the chemical nature of the substitution, its environment, its distance from the site, and the nature of the site residue(s) being affected.

Monoclonal antibodies against tumor markers

Identification of human brain tumor-associated markers would facilitate the development of new diagnostic and therapeutic strategies for these malignancies. The type III intermediate filament proteins (IFPs): vimentin, desmin and glial fibrillary acidic protein (GFAP), were studied in human glioma tissue extracts, in sera from glioma patients and in low passage glioma cell lines prepared from primary cultures of

freshly dissected tumors. Anti-GFAP, anti-desmin and anti-vimentin mAbs, showed high levels of these proteins in glioma extracts. Binding studies with authentic IFPs indicated the absence of circulating Abs against these proteins in the sera of glioma patients. On the other hand, these sera showed high levels of vimentin. Binding studies with these Abs using RIAs and western immunoblotting, showed that while anti-GFAF mAbs were specific to GFAP, anti-desmin mAb cross-reacted completely with GFAP, anti-vimentin mAb cross-reacted substantially with desmin and GFAP. Immunofluorescence staining of frozen sections revealed high levels of neurofilaments in gliomas and strikingly low levels in normal brain tissue. Double immunofluorescence staining showed co-occurrence of all three IFPs in the same filaments, suggesting either co-expression or cross-reactivity of these proteins due to their high degree of homology (27). Thus, caution should be exercised in interpretation of immunohistochemical data using Abs to IFs.The levels of several tumor-associated proteases, including plasminogen activators (PA), are elevated in many malignant tumors compared to their benign tumor counterparts. Our studies localized urokinase (UK) on the surfaces of breast cancer cells. anti-UK mAb concentrations exerted 50% inhibition of 3H-thymidine uptake by human breast cancer cell lines; Anti-UK mAbs exhibited little effect (10-20%) on normal human lymphocyte and liver cell lines. anti-UK MAbs had a potent cytolytic effect on human breast cancer cells. These results demonstrated the potential of antiUK mAbs as a valuable reagent for cancer immunotherapy and anti-metastatic therapy.

Our studies have confirmed the presence of large concentrations of various intermediate filament proteins (IFPs) in glioma tissue compared to normal brain. The monoclonal Abs against glial fibrillary acidic protein (GFAP) (anti-GFAP mAbs) recognized the cell surface of glioma cells and inhibition study showed that mAb B12B4 inhibited the proliferation of GB1 (96%), GB2 (85%) and AA (93%) at a concentration of 3.2 x 10(-10) M. One mAb (B12C4) inhibited the proliferation of GB1 (95%), GB2 (86%) and AA (94%) at a concentration of 3.26 x 10(-10) M and another mAb (B6C6) inhibited the proliferation of GB1 (75%), GB2 (75%) and AA (91%) at a concentration of 2.074 x 10(-10) M. We also demonstrated lysis of glioma cells after anti-GFAP mAbs treatment. Anti-GFAP mAbs had little effect (< or = 20%) on normal human lymphocyte, liver and intestine cell lines. These results were promising for radioimaging and immunotherapy of human gliomas.

Rabbit anti-UK polyclonal Abs and murine anti-UK monoclonal Abs were prepared by immunization with low molecular weight UK (LMW-UK) and high molecular weight urokinase (HMW-UK) synthetic peptide respectively. The polyclonal Ab cross-reacted with both LMW-UK and HMW-UK, whereas the murine mAbs were specific for HMW-UK.

Immunohistochemical study using anti-UK mAb demonstrated much higher levels of UK in glioma tissue than in normal brain antissue. Immunohistochemical study using anti-UK mAbs localized UK on the cell surface of glioma cells. Anti-UK mAbs inhibited the proliferation of AA cell lines and GB cell lines (50% to > 90%) and exerted minor effects (< or = 20%) on normal human liver, intestine and lymphocyte cell lines (28). The results showed the therapeutic potential for anti-UK mAbs against human gliomas and cancer metastasis.

Human chorionic gonadotropin, human thyrotropin receptor and insulin receptor

Five peptides corresponding to four regions of the beta chain of human chorionic gonadotropin (hCG), were synthesized, purified and characterized. The four regions were selected on the basis of sequence differences between the beta chain of hCG (beta hCG) and the beta chains of related hormones (29). The peptides bound rabbit and mouse anti-hCG Abs and rabbit anti-beta chain Abs, but did not bind Abs against the alpha chain or against other hormones. All the peptides, in their free form, elicited high titer antisera in rabbits and mice. Anti-peptide antisera bound to the immunizing peptide, to native hCG and to the isolated beta chain. These anti-peptide antisera did not bind to unrelated peptides, the alpha chain of hCG or to other hormones with very similar beta chains such as human luteotropic hormone (hLH), ovine luteotropic hormone (oLH) and equine chorionic gonadotropin (eCG). The areas represented by these peptides elicited Abs that are specific for human beta hCG and formulated the basis for the development of discriminatory reagents for the beta chain of hCG.

Two regions of human thyrotropin (thyroid-stimulating hormone, TSH) receptor (TSHR) (residues 12-44 and 308-364) were selected on the basis that they exhibit no sequence resemblance to luteinizing hormone/chorionic gonadotropin receptor. Five synthetic overlapping peptides (12-30, 24-44, 308-328, 324-344, and 339-364) were studied for their ability to bind 125I-labeled human TSH (hTSH), its isolated alpha and beta subunits, bovine TSH, ovine TSH, human luteinizing hormone, and human follicle-stimulating hormone. The human TSHR peptides 12-30 and 324-344 exhibited remarkable binding activity to human, bovine, and ovine TSH and to the beta chain of hTSH (30-32). We found that the binding of TSH to its receptor involves extensive contacts and that the TSHR peptides 12-30 and 324-344 contain specific binding regions for TSH that might be either independent sites or two faces (subsites) within a large binding site.

Seven regions of the alpha subunit of human insulin receptor (HIR) were synthesized and examined for

their binding of radioiodinated insulin (33). One peptide (namely, residues alpha 655-670) exhibited a specific binding activity for insulin. Binding curves of 125I-labeled insulin to adsorbents of peptide alpha 655-670 and of purified placental membrane were superimposable and completely inhibited by unlabeled insulin. The regions alpha 277-299 and alpha 705-731 contain autoantigenic sites of HIR, as they bound autoantibodies in a human serum of type 2 diabetes patients (34). In addition, region alpha 655-670 might constitute a minor autoantigenic site of HIR. Localization of these findings will permit the molecular investigation of the insulin-like activity of anti-HIR autoantibodies.

Botulinum neurotoxins

Molecular bases for immune recognition of botulinum neurotoxin, types A and B and the role of anti-toxin immune responses in defense against the toxin. We synthesized two sets of peptides, each was 92 peptides of 19-residues each, that overlapped by 5 residues and comprised an entire toxin (A or B). We determined the peptides' ability to bind anti-toxin Abs of human, mouse, horse and chicken (for review see ref 35). We also localized the epitopes recognized by Abs of cervical dystonia patients who developed immunoresistance to the correlate toxin during treatment with BoNT/A or BoNT/B (35). For BoNT/A, patients' blocking Abs bound to 13 regions (5 on L and 8 on H subunit) on the surface and the response to each region was under separate MHC control. The responses were defined by the structure of the antigen and by the MHC of the host (35). The antigenic regions coincided or overlapped with synaptosomes (SNPS) binding regions (35). Ab binding blocked the toxin's ability to bind to neuronal cells. In fact, selected synthetic peptides were able to inhibit the toxin's action in vivo (35). A combination of three synthetic strong antigenic peptides detected blocking Abs in 88% of immunoresistant patients' sera (35). Administration of selected epitopes, pre-linked at their N(α) group to monomethoxyploye thylene glycol, into mice with ongoing blocking anti-toxin Abs, reduced blocking Ab levels in the recipients (35). This may be suitable for clinical applications. Defined epitopes should also be valuable in synthetic vaccines design.

Myasthenia gravis

We found that autoimmunity could be manipulated by epitope-specific neonatal tolerance. For example, Neonatal tolerization of B6 mice with AChR or peptide alpha 146-162 followed by immunization with AChR in complete Freund adjuvant reduced incidence of clinical myasthenia gravis, indicating involvement of T-cell epitopes on alpha 146-162 in EAMG pathogenesis. But this is not really a practical method of treatment of an ongoing autoimmune disease. We also found that depression of autoimmune responses could be achieved by injection with tolerogen (monomethoxypolyethylene glycol)-conjugated pathogenic auto-epitopes after autoimmunity develops. In autoimmune disease, production of diseasecausing auto-Abs depends on autoreactive T cells that recognize the epitopes of the pathogenic antigen in the context of MHC class II molecules. It was possible that selective inhibition of an antigen-presenting function of disease-associated MHC alleles could lead to suppression of the disease. Myasthenia gravis (MG) is a disabling neuromuscular disease in which autoimmune responses, primarily against acetylcholine receptor (AChR), especially against the alpha chain of AChR, or less frequently, against muscle-specific kinase (36), cause a postsynaptic defect. HLA linkage of MG has been thus far best detailed for DQB1 (37). Recently, we have shown that certain DQ haplotypes are associated with presentation of AChR alpha-chain peptides in MG (38). In a mouse model for MG, which can be induced in disease-susceptible C57BL/6 (B6, H-2b) mice by injection with Torpedo AChR, region 62-76 of I-Ab beta chain is involved in the disease mechanism (39). Monoclonal Abs (mAbs) against synthetic peptide I-Abetab62-76, which localizes at the rim of the antigen-binding site of I-Ab, inhibited in vitro proliferation of disease-associated T cells (37,40). Passive transfer of these mAbs as well as vaccination with this peptide strongly suppressed occurrence of clinical MG in B6 mice (40). In both cases, Ab and T-cell responses against AChR, especially those related to disease pathogenesis, also decreased (41). mAbs against peptides from the ridge of the antigen-binding region of the correlate DQB1 sequences inhibited in vitro the proliferation of AChR-specific T cells from MG patients (37). The results indicated that the function of disease-associated MHC alleles may be blocked by directly and selectively targeting the antigen-presenting region on these MHC molecules (42). The strategy could provide an effective means for immune intervention in other autoimmune and allergic responses.

Recently, we humanized a murine mAb, (LG11), capable of blocking MG-associated DQ beta 1 (DQB1) allele and reformatted it into single-chain fragment variable (scFv) (43). A fully functional humanized scFv was obtained by optimizing variable domain orientations and linker lengths, along with the optimization of expression conditions and codons to suit Escherichia coli expression machinery. Characterization of humanized scFv (FL8) revealed that the reformatted scFv, despite recognizing the same epitope as the parent murine LG11 mAb, exhibited superior binding affinity (0.97 nM) compared to the LG11 mAb, towards the immunizing antigen (DQB1*0601/70-90) and was able to block the proliferation of T cells cultured from

PBLs of MG-patients typed DQB1*0601. The scFv was also capable of binding a variant MG-associated allele (DQB1*0502/70-90) with moderate affinity (18.7 nM), a feature that was absent in the LG11. To our knowledge, this is the first report of humanizing a MG-associated human leukocyte antigen (HLA) scFv for preclinical studies.

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Understanding and Applying Glass

by Yuanzheng Yue, Member EUAS

Short Biography

Dr. Yuanzheng Yue is Professor of Chemistry at Aalborg University, Denmark. He is the founder of the inorganic glass research laboratory in Denmark, and the head of Center for Amorphous Materials Science. He is a distinguished visiting professor at Wuhan University of Technology and Qilu University of Technology, China. In 1995, he received his Ph.D. degree at Berlin University of Technology, Germany. His research areas include glass science, glass fiber technology, metallic glasses, amorphous materials for thermal insulation, energy storage and membrane, and metal-organic framework glasses. He is the author/co-author of more than 280 papers in peer-refereed journals, and delivered about 100 invited and plenary talks at international conferences. In 2014, he was awarded Knight's Cross of the Order of the Dannebrog in Denmark. He is an editor of Eur. J. Glass Sci. Techn., and an editorial board member of J. Non-Cryst. Solids, and an associate editor of Frontiers in Materials (Glass Section). He is a council member of the International Commission on Glass (ICG), and the founding chair of the ICG Technical Committee for Glass Fibres.

Over the past three decades, Yue and his group have been working in the field of materials science with emphasis on glass science and technology. His key scientific contributions to glass science and technology include the following 10 aspects.

1. Glass Relaxation and Glass Ttransition

By performing extensive experimentations and theoretical studies, Yue established a general, accurate approach for understanding the glass transition and relaxation in glasses with various thermal and mechanical histories. The approach is based on the sequence of the experiments: hyperquenching, sub-T_g annealing, differential scanning calorimetric (DSC) scanning, structural analysis and modelling. Through this approach, Yue, in collaboration with his collaborators, have achieved several discoveries that are crucial for exploring the nature of glass-forming liquids in terms of the potential energy landscape [*Nature 2004, Appl. Phys. Lett. 2002, J. Phys. Cond. Mat. 2003, J. Phys. Chem. B 2008*]. They found that the structural and energetic heterogeneities exist in all the studied glasses and supercooled liquids, but the extent and type of structural heterogeneity depends on the glass chemical composition and the liquid fragility. They succeeded in modelling the sub-T_g enthalpy relaxation behaviour of both the hyperquenched (HQ) and the annealed HQ glasses by establishing a composite stretching function [*Chem. Phys. Lett. 2010*]. They revealed the origin of the excess density of vibrational states in glass [*Phys. Rev. Lett. 2006, 2008, 2014*]. They developed a simple DSC approach, by which the fictive temperature of a hyperquenched glass can be determined. Yue established an integrated

calorimetry-viscometry approach for determining any cooling rates that a liquid undergoes during his formation. This approach has widely been applied in quantifying mechanical and thermal histories of glass fibres, metallic glasses and natural glasses.

2. Dynamics and Rheology of Glass-Forming Liquids

Yue and Brückner achieved several breakthroughs in studying the non-linear flow behaviour of glass melts during deformation, and established a phenomenological model that accurately describes the non-Newtonian flow of inorganic glass melts. They developed a numerical approach, by which the heat-dissipation effect could be separated from the total viscosity decrease in glass melts caused by uniaxial compression. They clarified the correlations between glass composition, structure, non-Newtonian behaviour, and melt workability. Yue is a co-author of the paper that reports a new three-parameter viscosity model, namely, the Mauro-Yue-Ellison-Allan-Gupta (MYEGA) model. The model accurately describes the entire viscosity-temperature relation for both inorganic and organic liquids. Yue initiated a systematic study of anomalous dynamics of metallic glass forming liquids (MGFLs). He and his co-authors discovered a universal dynamic feature of these liquids, namely, the fragile-to-strong phase transition in many types of MGFLs. Furthermore, Yue has provided insight into the correlation between the iso-structural viscosity, configurational entropy, and fragility of glass-forming liquids.

3. Mechanical Properties of Glass and Glass Fibres

Yue's group has clarified a long-standing question why a glass fibre exhibits significantly higher tensile strength than its counterpart bulk glass with same chemical composition (*J. Am. Ceram. Soc. 2008, 2010*). The experimental evidence was achieved by comparing the tensile strength of continuous glass fibres with that of glass wool fibres for same diameter and composition, but different drawing forces that both types of fibres were subjected to. The results show that the drawing force induced structural anisotropy, i.e., orientation of structural units, and thereby enhanced the tensile strength of glass fibres. Besides the structural anisotropy, defect orientation and surface characteristics also play an important role in affecting the fibre strength. They discoved the fracture mechanism and fracture pattern of glass fibres. They demonstrated the impact of the fictive temperature on mechanical properties such as elastic modulus and hardness by performing the nano-indentation directly on thin glass fibres (first time ever) (*J. Non-Cryst. Solids* 2008). Smedskjaer, Mauro and Yue succeeded in predicting glass hardness by using the temperature dependent constraint model (a highlighted paper in *PRL* 2010).

4. Multi-functional Glasses by Inward Diffusion

Yue proposed the concept of initiating the inward ion diffusion in glass in a reducing atmosphere at temperatures around the glass transition temperature T_g, thereby to create a silica nanolayer on glass surfaces. His former student Morten M. Smedskjaer and Yue implemented this concept, and thereby enhancing the mechanical and chemical performances, and generating new photonic functionalities (*Chem. Mater. 2009, Appl. Phys. Lett. 2011, J. Mater. Chem. 2011*). The main factors influencing the inward ion diffusion are the selection of polyvalent ions, reducing gases, and heat-treatment temperature and duration. Their findings related to the inward diffusion have contributed to understanding of glass problems such as liquid fragility, glass structure topology and transport properties) (*J. Phys. Chem. B, 2009 and J. Chem. Phys., 2009*).

5. Glass Structure

Yue's group found the NMR evidence for the local structural alignment of metaphosphate glasses that were subjected to mechanical deformation (extrusion) (JNCS

1998). They also obtained the evidence of the structural heterogeneity in calcium aluminosilicate glasses by performing NMR and modeling approach (*Chem. Mater*. 2010). The correlations among structure, property, and glass-forming ability in boroaluminosilicate glasses were clarified (*Phys. Rev. B 2012, J. Non-Cryst. Solids 2012, Appl. Phys. Lett. 2012*).

6. Glass in Cement

Yue's group has made substantial progress in applying glass materials to develop environmental friendly cement products for future. They succeeded in designing the glass compositions that could substitute 20% of clinker. By doing so, the amount of clinker in cement products will be reduced so that CO_2 emission can be greatly reduced since the major raw materials for producing clinker is limestone that release CO_2 upon calcination. The glass particles are pozzolanic and also enhance the compressive strength of the final cement with help of additional limestone (*J. Am. Ceram. Soc.* 2012).

7. Insulation Amorphous Materials

Over the past two decades, Yue's group has carried out extensive research on insulation amorphous materials including stone wool fibers and glass foams. Through their research, a solid knowledge basis has been built for glass fiberizing and glass foaming technology. The performances of both stone wool and glass foams have been greatly improved (*J. Am. Ceram. Soc.* 2009, *Ceram. Int.* 2015).

8. Discovery of Metal-Organic Framework (MOF) Glasses

Yue and his collaborators discovered the fourth and completely new family of melt-quenched glasses (MQGs): hybrid metal-organic framework bulk glasses, in contrast to other three inorganic non-metallic glass, organic glass, and metallic glass (*Nat. Commun.* 2015). It is shown that some of the zeolitic imidazolatee frameworks (ZIFs) (a subset of MOFs) can be melted and vitrified. The ZIF glasses could be obtained by an optimum design of chemical compositions, well-controlled dynamic heating and cooling processes. Remarkably, by using DSC, they observed the polyamorphic transition in ZIF-4 crystals, i.e., the transition from the low density to the high-density amorphous phase and co-existence of the two phases at a certain temperature. They found the ZIF glasses are extremely stable against crystallization (*Sci. Adv*. 2018). This discovery provides deep insights into the glass transition, polyamorphic transition, collaborative melting, glass crystallization, liquid fragility.

9. Enhancing the Lithium Ion Battery Performances by Order/Disorder Engineering

The performance of the anode materials is critical to further development of Li-ion batteries. However, the cycling stability and safety performance of anode materials are still far from satisfying. Therefore, Yue-Zhang group proposed a new strategy, i.e., the disorder/order engineering, by which the performances of the Li-ion batteries can be greatly improved. First, the disordered materials, i.e., glasses, were prepared by vitrifying V_2O_5-TeO_2 (VT) liquids, and then the VT glass powder was mixed with acetylene black and binder to form anode for a lithium ion battery. Second, by subjecting the battery to discharging/charging cycles, the VT glass was partially transformed into ordered phases, i.e., nanocrystal formation via the disorder-order transition. Even the first few cycles of discharging/charging could induce the disorder-order transition. The ordered nano-domains and the disordered matrix exert a synergetic effect to facilitate the ionic and electronic transport and to maintain structure stable against discharging/charging. As a consequence, both the capacity and the cycling stability were greatly enhanced (*Nano Energy* 2018). This finding has opened a new way for developing high performance anodes for Li-ion

batteries.

10. Clarifying the Origin of the Ion-Insertion Induced Nanocrystal Formation

As described above, Yue-Zhang group found that nanocrystals could be generated in glass anodes by Li-ion insertion, and thereby the cycling stability of Li-ion batteries was enhanced. This type of crystallization has never been reported in literature. Here the key question arises: What are the mechanisms of both the nanocrystal formation and the enhancement of battery performances. Very recently, Yue-Zhang group has answered this question to large extent by exploring phase transitions, redox reactions, and structural heterogeneity in glass anodes (*Nano Energy* 2019). Li ions interact with the higher energy domains of structural network during discharging/charging, some of those ions are incorporated into the structural network, and thereby the potential energy is lowered through nanocrystal formation. The nanocrystals in $40TeO_2$–$60V_2O_5$ glass were identified to be γ-Li_3VO_4. Owing to the metastable nature of the γ-Li_3VO_4 phase, the glass anode becomes electrochemically active and highly ionic conductive. Simultaneously, the cycling stability is greatly enhanced by the nanostructured glass.

Representative papers

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Metals and Materials Utilisation and Applications Research

by Herman Potgieter, Member EUAS

Short Biography

***Current position**: Head of School, School of Chemical and Metallurgical Engineering, University of the Witwatersrand, Johannesburg, South Africa. Joint position as Professor of Waste Beneficiation and Transformation, Faculty of Science and Engineering, Manchester Metropolitan University, Manchester, UK*

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1980 – B.Sc. Hons. (Chemistry)
1981 – M.Sc. Chemistry
1986 – B.Sc. Hons. (Water & Environmental Sci. & Eng.)
1996 – Ph.D. Eng. (Metallurgy and Materials Engineering)
2003 – Doc. Tech. Applied Chemistry

Professional registration, membership and service
Fellow IOM3 (Institute of Materials, Minerals and Mining), CEng.
Fellow RSC (Royal Society of Chemistry), CChem
Associate Editor – Corrosion Engineering, Science and Technology
Editorial board member Journal of the Southern African Institute of Mining and Metallurgy, SA Journal of Science and Technology, African Corrosion Journal, Journal of Hazardous Materials (until 2015), Journal of Radioanalytical and Nuclear Chemistry (until 2016)

Research
Professor Potgieter has worked 13 years in private industry and the remainder of his career in academia. To date he has supervised 50 master's and doctoral degree students to successful completion of their degrees, and published more than 200 peer-reviewed journal articles and conference proceedings, as well as 5 book chapters. He also had almost 50 published conference contributions and nearly 30 popular scientific and technical papers to his credit. His research spans the general area of materials utilisation and applications, and he has made numerous contributions to the areas of waste materials utilisation, water treatment, cement and concrete research, metals extraction and beneficiation and corrosion of alloys containing PGMs (platinum group metals) in reducing acids and other aggressive process environments. The projects undertaken all had a practical, problem solving focus to be of use and value to the industry.

(1) Waste Materials Utilisation and Applications

Coal fly ash is a by-product of coal combustion in coal fired power stations and an industrial waste which is produced in large tonnages all over the world. In South Africa, which relies for more than 90% of its energy needs from coal, either as electrical power or as raw material for synthetic fuel, approximately 35 million tonnes of coal fly ash is produced annually, while worldwide the figure is between 650 – 700 million tonnes. Its

main application is as a mineral addition to cement and concrete, where it has several advantages in terms of the workability of the concrete and can be utilised to reduce the greenhouse gas emissions associated with cement production. However, this only accounts for 10-25% use of its production, depending on the country considered, and large amounts remain as landfill dumps with the associated problems of producing leachate which is harmful to the environment and groundwater resources, not to mention the space it occupies.

Research in this area by prof. Potgieter and his co-workers has focused on the application of fly ash in water treatment as an adsorbent for, amongst other things, phosphates, heavy metals, phenolic compounds and colourants from the dye industry. Because coal fly ash typically consists of almost a third of Al_2O_3 (alumina) in a glassy matrix, it is an excellent replacement for bauxite ores to produce aluminium from, provided that an economically feasible process for its recovery and extraction can be developed, and this is one of the focus areas of the current work in the group. The application of fly ash in refractory materials and as a constituent of mine backfill paste have also received attention as alternative avenues to consume larger volumes of waste coal fly ash.

A promising area for the consumption of coal fly ash is in the polymer industry. The addition of coal fly ash as a mineral filler in several polymer-type products, can substantially enhance the wear resistance, flow behaviour and mechanical strength of polymeric materials. Most work to date has concentrated on polypropylene, and other polymer matrices are currently under consideration to extend this work to. One of the very successful applications of fly ash in polypropylene was in a rota-moulding application, which is a process for producing hollow polymer products like drums and canoes, for example. Further work is underway to determine the role of plasticisers and coupling agents in this process and optimising their usage in conjunction with fly ash fillers.

(2) Improving the Corrosion of Stainless Steels under Reducing Acid Process Conditions

Stainless steels are famous for their corrosion resistance against oxidising acids like nitric acid. This resistance stems from a very thin, but tenacious oxide film on the surface of the stainless steel. When this film is compromised, or the material is exposed to reducing conditions, which are not conducive to the repair of the passive film, corrosion damage of the stainless steels can be quite dramatic. By adding a small amount of a PGM (platinum group metal) to stainless steels, the corrosion resistance under reducing conditions can be substantially increased. This phenomenon is known as the “cathodic modification” effect, and relies on the increased ease of hydrogen evolution from the material’s surface and consequently a change in the rate of the cathodic reaction. Under favourable conditions this can increase the corrosion potential of the stainless steel to a value in the passive potential range and hence a large decrease in the corrosion current and rate. The cathodic modification effect was developed by a group of Russian researchers between 1948 to the late 1970’s, with a few ad hoc contributions by some other groups in the USA.

Work by Prof. Potgieter and his co-workers involved the investigation of the corrosion resistance and behaviour of various types of stainless steel alloys in both sulphuric and

hydrochloric acids at different concentrations and temperatures and with various PGM elements. Most of the work published since the early 1980's came from Prof. Potgieter's group, initially at Mintek (Council for Minerals Technology) and later the University of the Witwatersrand in South Africa. The research confirmed and discovered several interesting facts, such as the fact that:

(i) the corrosion resistance of ferritic stainless steels are enhanced to a much larger degree by a small PGM addition than in the case of austenitic stainless steels.
(ii) the corrosion behaviour duplex stainless with PGM additions is not a simple summation combination of that of ferritic and austenitic stainless steels with PGM additions
(iii) the efficiency of the cathodic modification effect is dependent on the type of PGM used and regardless of which type of PGM that is used, is more effective in sulphuric acid than hydrochloric acid
(iv) there are several synergistic effects between PGM additions and elements like Mo and Ni in the stainless steel which enhanced the corrosion resistance to a larger degree than any one element on its own
(v) too small an amount of PGM element to establish the cathodic modification effect effectively, actually accelerates the corrosion rate more than when it is not present at all.
(vi) this phenomenon also worked very well in titanium alloys
(vii) surface modification of an alloys by a PGM element, whether plated, PVD (physical vapour deposition) deposited or applied by laser surface alloying, are all equally effective as long as a certain minimum amount of PGM is present
(viii) some PGMs not only affect the cathodic part of the corrosion reaction, but also inhibits the anodic dissolution part to various extents
(ix) the PGM element, if it is Ru, gets incorporated into the passive film which forms on the surface of the stainless steel or titanium alloy during passivation.
(x) the PGM additions also increase the pitting corrosion resistance of alloys in chloride media

Further research in this area is ongoing and has recently be extended to copper alloys.

(3) Novel Methods of Extracting Metals from Low Grade Ores and Wastes

The latest research by prof. Potgieter and his co-worker is focused on new and novel ways to extract various metals from low-grade ores and waste. In this regard three separate but related technologies are pursued:

(a) Using supercritical carbon dioxide containing a dissolved ligand for the extraction of metals from different matrices. A high pressure reactor is used and the supercritical carbon dioxide containing a dissolved ligand (usually an organic type compound) is pumped to flow through a porous packed bed of finely ground ore or waste material. The dissolved ligand can be tailored to react selectively with only one of the metals in the ore/waste or with a number of them. The ligand-metal complex is the carried in a dissolved state in the supercritical carbon dioxide medium out of the reactor and collected in a separate reactor. Here the pressure is lowered and the ligand-metal complex recovered. The metal can then be further

refined though precipitation, electrowinning or selective reduction, while the ligand is regenerated to be recycled through the process.

(b) Gas phase extraction of metals from low-grade ore or waste in a fluidised bed reactor using a volatile ligand. The ligand is volatilised and fed together with a supporting gas stream into a reactor containing the pulverised low-grade ore, or waste, to fluidise the bed. In this process the ligand, which can again be tailored for selectivity, reacts with the metal, and the volatile ligand-metal complex which forms, is carried in the gas stream out of the reactor and through a condenser to recover it as a liquid. From this liquid the metal can be recovered and the ligand recycled to the front end of the process. The processes investigate to date operated at temperatures of between 180 – 250 ^{o}C and have proven very successful for several metals such as Fe, V and Al, but less so for Cr. This implies that it can potentially be tailored to achieve selective separation processes for certain metals. Work is in the very early stages, but some promising results have been achieved to date and much more research is planned in this area.

(c) The final area of research is the use of ionic liquids, in a process which has lately been termed ionometallurgy by some workers in the field. Once again additional ligands can be included in the ionic liquids, or the ionic liquids can be used on their own to dissolve selected metals from a variety of matrices. While groups in the UK and Belgium have already reported a large number of investigations of using ionic liquids for (selective) metal dissolution from a number of matrices, the work in prof. Potgieter's group focuses on practical applications to leach metals from real life waste materials and low grade ores. The ability to also tailor ionic liquids by either their design or dissolving addition reductants/oxidisers in them, creates vast opportunities for practical applications, e,g. recovering high value metals from metallurgical or consumer waste streams. While a recent addition to the group's areas of research, work is slowly starting to emerge to indicate that this area holds much promise for the future.

From Nano to Macro: A Few Lessons Learned from Materials Research

by Yang-Tse Cheng, Member EUAS

Short Biography

Education History

Physics, Peking University, 1978-1980; B.S., Physics and Mathematics (with Honor), Caltech, 1982; M.S., Applied Physics, Caltech, 1983; Ph.D., Applied Physics, Caltech, 1987. PhD thesis title: "Ion-beam mixing and the formation of amorphous alloys" and thesis advisors: William L. Johnson and Marc-Aurele Nicolet.

Work History

General Motors R&D Center: Senior Research Scientist (1987 - 1992), Staff Research Scientist (1992-2001), Senior Staff Research Scientist (2001 - 2004), GM Technical Fellow (2004 - July 2008); Laboratory Group Manager, Engineered Surfaces and Tribology (1999 - 2003), Laboratory Group Manager, Engineered Surfaces and Functional Materials (2003 - Dec. 2006).

University of Kentucky: Professor of Materials Engineering (August 2008 - present), Frank J. Derbyshire Professor of Materials Science (June 2011 - present), Professor (joint appointment) of Physics and Astronomy (June 2015 - present).

Honors and Awards

- *Member, EU Academy of Sciences (EUAS) (2018)*
- *Fellow, National Academy of Inventors (2017)*
- *Fellow, Materials Research Society (2013)*
- *Fellow, American Physical Society (2005)*
- *John M. Campbell Award, "Modeling Micro- and Nano-indentation Measurements" (2005); Charles L. McCuen Award, "Hard Coatings for High Power Density Transmission Gears" (2005); John M. Campbell Award, "Synthesis and Theory of Novel Surface-Modified Materials" (1995); General Motors R&D Center.*
- *R. F. Bunshah Award, American Vacuum Society, for best paper on "What is indentation hardness?" presented at the International Conference on Metallurgical Coatings and Thin Films (2001)*
- *Graduate Student Award, Materials Research Society (1987)*

Summary of Research Activities

YT Cheng is most grateful for the opportunities afforded him in his personal and professional life. His parents, two highly acclaimed scientists, introduced him to math and science early in his childhood. As a graduate student, he worked on a cross-disciplinary topic under the supervision of two distinguished professors. At General Motors R&D Center, he was exposed to a wide range of interesting and challenging materials research topics which led to his investigations into the nano- and micro-meter scale behavior of materials and their applications, such as nanoindentation modeling and measurements of mechanical properties; growth, structure, and properties of nanostructured materials (e.g., amorphous materials, nano-composites, epitaxial single crystals, single crystal nanowires); microscopic shape memory and superelastic effects; magnetorheological fluids; superhydrophobic and superhydrophilic surfaces; ion-solid interactions and ion beam modification of materials; automotive applications of new materials and processes,

including electrical contacts, high power-density engines and transmissions, environmentally friendly machining processes, hydrogen sensors, fuel cells, metal hydride batteries, and lithium ion batteries. Presently, he is focusing on training graduate students through research at the intersection of mechanical and electrochemical behavior of materials for developing better batteries for electric vehicles. Cheng's research activities have been documented in 8 edited books and special volumes, 180 publications, and 48 issued US patents.

Thermodynamic and fractal geometric aspects of ion-solid interactions
Yang-Tse Cheng, Materials Science Reports 5 (2), 45-97 (1990).

Abstract: A thermodynamic approach to atomic diffusion in a thermal spike is reviewed. The approach is based on recent ion mixing experiments which demonstrate the influence of the heat of mixing and the cohesive energy of solids on ion mixing. These thermodynamic effects are assimilated into a phenomenological model of ion mixing. The model is generalized to low-energy ion mixing during sputter depth profiling and is used to elucidate the nature of atomic diffusion in a thermal spike. The onset of radiation-enhanced diffusion in ion mixing is also discussed. A fractal geometry approach to spike formation is presented. An "idealized" collision cascade constructed from the inverse-power potential $V(r) \propto r^{-1/m}$ $(0 < m \leq 1)$ is shown to have a fractal tree structure with a fractal dimension $D = 1/2m$. The same fractal dimension can also be derived from the Winterbon-Sigmund-Sanders (WSS) theory of atomic collisions in solids. The fractal dimension is shown to increase as an actual collision cascade evolves, because of the change of the effective interaction potentials. The concept of "space-filling" fractals is used to specify spikes. The formation of local spikes, their energy densities, the probability of local spikes overlapping, and the time evolution of a collision cascade are also investigated. It is shown that spikes are not expected to form in a single-component solid consisting of elements with atomic number less than 20; many-body collisions have little effect on the formation of spikes; and, the similarity between high-and low-energy ion mixing is the result of the fractal nature of collision cascades.

Background and relevance of this work: A fundamental understanding of ion-solid interactions is important to several industries, such as ion implantation for semiconductor device fabrication, ion beam modification of materials for improved corrosion and wear resistance, and radiation damage prevention in nuclear power plants. Under the guidance of Professors W. L. Johnson and M.-A. Nicolet, Cheng and collaborators demonstrated the importance of thermodynamic driving forces in ion beam mixing and proposed a fractal geometric model to describe the evolution of collision cascades to thermal spikes. At GM R&D Center, Cheng realized that similar thermodynamic effects exist during sputter-depth profiling, a widely used technique for measuring the concentration profiles of materials near surfaces and across interfaces. Today, the thermodynamic effects and the fractal approach are well established and are highlighted in several textbooks and monographs on ion-solid interactions, ion beam modification of materials, and radiation effects.

Relationships between hardness, elastic modulus, and the work of indentation
Yang-Tse Cheng and Che-Min Cheng, Applied Physics Letters 73 (5), 614-616 (1998).

Abstract: The work done during indentation is examined using dimensional analysis and

finite element calculations for conical indentation in elastic-plastic solids with work hardening. An approximate relationship between the ratio of hardness to elastic modulus and the ratio of irreversible work to total work in indentation is found. Consequently, the ratio of hardness to elastic modulus may be obtained directly from measuring the work of indentation. Together with a well-known relationship between elastic modulus, initial unloading slope, and contact area, a new method is then suggested for estimating the hardness and modulus of solids using instrumented indentation with conical or pyramidal indenters.

Background and relevance of this work: Cheng became interested in measuring the mechanical properties of thin films and coatings because of several automotive applications, such as tool coatings for dry machining, tribological coatings to increase the contact fatigue life of gears used in automobile transmissions, and coatings for piston rings and fuel injectors. Nanoindentation was and has been one of the few available techniques to measure the mechanical properties of thin films and coatings. Cheng and his father, Dr. Che-Min Cheng (Zheng Zhemin), wrote a series of papers using dimensional analysis and finite element calculations to investigate the possibilities and limitations of nano- and micro-indentation. This paper established a relationship between material's hardness, elastic modulus, and the work of indentation (i.e., the areas under the respective loading and un-loading curves). This relationship provides an energy-based interpretation to what hardness is and how to measure it.

Recovery of microindents in a nickel–titanium shape-memory alloy: A "self-healing" effect
Wangyang Ni, Yang-Tse Cheng, and David S. Grummon, Applied Physics Letters 80 (18), 3310-3312 (2002).

Abstract: The thermally induced recovery of microscopic deformation in a nickel–titanium shape-memory alloy was examined. Surface deformation was simulated by indenting the alloy in the martensite phase at room temperature using both spherical and pyramidal indenters. We show that deformation in spherical microindents can be almost completely reversed by moderate heating. Partial recovery was observed for pyramidal impressions formed by a Vickers indenter and the recovery ratio was independent of the indentation depth. The observations were rationalized using the concept of representative strain and maximum stress under the spherical and pyramidal indenters.

Background and relevance of this work: Shape memory alloys were known to have the ability to "remember" and return, upon heating, to their original shapes after being deformed by tension, compression, or shear. It was unclear, however, whether the shape memory behavior could be exploited for self-healing of scratches and indents encountered in many situations (e.g., scratches on the body panel of automobiles or on the cylinder wall after running the internal combustion engine in extremely cold conditions). Intrigued by the potential applications of shape memory materials for self-healing of scratches and indents, Cheng and collaborators investigated micro- and nano-scale shape memory behavior under complex loading conditions such as spherical and pyramidal indentations. Their work showed that both one-way and two-way shape memory behavior exist even at the nano-meter length scale, leading to the possibility of using these shape memory surfaces for healing damages, storing information, and controlling friction, wetting, and heat transfer.

Is the lotus leaf superhydrophobic?
Yang-Tse Cheng and Daniel E. Rodak, Applied Physics Letters 86 (14), 144101 (2005).

Abstract: Superhydrophobic surfaces have important technical applications ranging from self-cleaning window glasses, paints, and fabrics to low-friction surfaces. The archetype superhydrophobic surface is that of the lotus leaf. When rain falls on lotus leaves, water beads up with a contact angle in the superhydrophobic range of about 160°. The water drops promptly roll off the leaves collecting dirt along the way. This lotus effect has, in recent years, stimulated much research effort worldwide in the fabrication of surfaces with superhydrophobicity. But, is the lotus surface truly superhydrophobic? This work shows that the lotus leaves can be either hydrophobic or hydrophilic, depending on how the water gets on to their surfaces. This finding has significant ramifications on how to make and use superhydrophobic surfaces.

Background and relevance of this work: While searching for an efficient way of removing water, which is a byproduct of hydrogen fuel cell engines, Cheng and co-workers realized that previous studies of "superhydrophobic" surfaces were mostly done by placing or splashing water drops on surfaces to observe the contact angle and rolling behavior of the drops. However, water vapor is present in the fuel cells. Do water drops formed by vapor condensation also have high contact angle and rolling behavior on "superhydrophobic" surfaces? This paper addressed this question which stimulated further investigations into the mechanisms of superhydrophobicity.

The influence of surface mechanics on diffusion induced stresses within spherical nanoparticles
Yang-Tse Cheng and Mark W. Verbrugge, Journal of Applied Physics 104 (8), 083521 (2008).

Abstract: We examine the effects of surface tension and surface modulus on diffusion-induced stresses within spherical nanoparticles. We show that both the magnitude and distribution of stresses can be significantly affected by surface mechanics if the particle diameter is in the nanometer range. In particular, a tensile state of stress may be significantly reduced in magnitude or even be reverted to a state of compressive stress with decreasing particle radius. This reduction in tensile stress may be responsible for the observed resilience to fracture and decrepitation of nanoparticles used in various industrial applications.

Background and relevance of this work: Advanced lithium ion battery electrodes experience large volume changes caused by concentration changes within the host particles during charging and discharging. Electrode failure, in the form of fracture or decrepitation, can occur as a result of repeated volume changes. This paper showed why electrodes made of nanoparticles were less likely to crack. In a series of subsequent publications, Cheng and co-workers proposed an electrochemical Biot number, which could be used to characterize stress and strain energy evolution in an electrode. They also proposed tensile stress and strain energy based criteria for the initiation and propagation of cracks in electrodes. These criteria have helped guide the development of new materials for lithium ion batteries with high energy density and long cycle life.

Oil, Gas & LNG Construction and Project Management

by Xiangyu Wang, Member EUAS

Short Biography

Work Experience

Professor (Personal Chair) (2011 to presence), Curtin University, Australia
Curtin-Woodside Chair Professor for Oil, Gas & LNG Construction and Project Management (July 2013-July 2018), Curtin University, Australia
College of Experts, ARC (Australian Research Council) (January 2016 – Dec 2018), Australian Government
Acting Woodside Chair Professor of LNG Construction (February 2012 – July 2013), Curtin University, Australia
Curtin Director of Australasian Research Centre for Building Information Modelling (BIM) (March 2012 - presence), Curtin University, Australia
Editor-in-Chief, Visualization in Engineering: an International Journal, Springer-Verlag (2012 - presence)

Education

Ph.D., Purdue University, 2005
Master, University of Washington, 2002
Bachelor, Tongji University, 2000

Recognitions

Member, EU Academy of Sciences, since 2018
Keynote and Plenary Speakers for over 50 International conferences/forums
World Top 100 Engineers, 2014
External judge for Innovation and Technology award, 2013 Woodside Awards
The impact of his work was reported over 40 times by a wide range of international and domestic prestigious media. His work with his industry partners was featured twice in the Australian newspaper, Energynewsbulleting.net, *ScienceWA magazine, LNG World News, Business News, Western Australian Energy Research Alliance, CNN, the Conversation, and Energy Publications*
Editor-in-chief, Visualization in Engineering: an International Research Journal, Springer Verlag
Editorial Board Member, Journal of Construction Engineering and Management, American Society of Civil Engineers (ASCE) (2007-present), Journal of Information Technology in Construction (ITcon), Engineering, Construction and Architectural Management (ECAM), since 2015, The Open Construction and Building Technology Journal, Bentham Science Publisher, since 2011, Journal of Frontiers in Construction Engineering (FCE), since 2012, Journal of Construction Engineering, Science and Engineering Publishing Company, since 2012, International Journal of Oil and Gas, since 2014, Journal of Frontiers of Information and Communication Technology, since 2014
Guest Editor, Automation in Construction, Elsevier, 2009, 2012, 2013, 2014, Journal of Operational Research Society, 2012, Journal of Information Technology in Construction (ITcon) 2012, 2014, International Journal of Advanced Robotic Systems, 2012, Journal of Industrial and Management Optimization, 2013, 2014, Archives of Computational Methods in Engineering, 2014, Journal of Intelligent and Robotic Systems, 2014, Scientific World Journal, 2014.
Book Editor, for over 10 books for Springer Verlag, Wiley, IGI Global, and Bentham eBook

SUMMARY OF IMPACT

As an industry chair and a university professor, Prof Wang pioneered and implemented digital technologies into practices to significantly improve asset life cycle performance. By creating a nexus between industry and research, he has established a continuing dialogue that broadens opportunities for tangible and measurable innovation. The created best practices are widely disseminated via a reputable industry-focused innovation ecosystem which Prof Wang is running, and are becoming industry standards at various levels. Those enabling technologies and best practices are transforming our industry by shaping construction and capital projects' digital future.

Industry impact of his innovation is highlighted by his establishment and leadership of a reputable industry alliance where he has been closely working with over 50 industry partners for knowledge creation, translation, dissemination, and standardization. The alliance and its innovation and industry practices have proved to improve productivity in building, infrastructure, minerals and energy industry sectors. Tons of evidences can be found in the 40 times of media report, and industry leaders' acknowledgement letters.

His academic achievements are highlighted by over 300 top tier refereed journal articles in various disciplines and inter-disciplines. His Google Scholar Citation is close to 6,000 with an H-index nearly 40. He has successfully delivered over USD $20 million innovation, research, and industry best practice projects funded by the industry alliance, Australian Research Council, US National Science Foundation, Korean NRF, China Natural NSF grants, etc.

After working as a Post-doc Research Associate, Lecturer, and Senior Lecturer for a couple of years, Prof. Wang was offered a personal chair Professor with 100% time research in July 2011 by the School of Built Environment at Curtin University. Since March 2012, he has taken the role of directing Australasian Joint Research Centre for BIM. Prof. Wang's major roles are research (80%) and administration (20%) without teaching duty as a research professor. He spends 80% of his time researching ARC projects, supervising PhD students, and writing research papers. He spends about 20% of his time leading the Australasian Joint Research Centre for BIM to attract more ARC grants, publish high quality papers, and train research students.

As a remarkable recognition for his excellent performance, Prof Wang was nominated by Curtin as the Curtin-Woodside Chair for Oil, Gas and LNG Construction and Project Management since July 2013. Meanwhile, he is also the Director of Program 3 "Productivity through Innovation" under the Sustainable Built Environment national research centre (SBEnrc) which has an extensive connection with Australian industry in terms of research projects. He is the Steering Committee Member and "Marine BIM" Research Program Leader of the Joint Research Centre for Marine, Sub-sea and Ocean Engineering and Technology (Curtin University and Ocean University of China) since 2014.

Prof. Wang's research interests focus mainly on BIM, visualization and Information Technology in Construction Engineering and Management, Facilities. The BIM Centre, for which Prof. Wang is the Director, has created an industrial alliance with 40+ members from owners, contractors, consultants, and technology providers.
Some key facts about the BIM Centre are:

- More than **USD $ 20 million** research funding in the past five years, including overall 12 ARC grants which consist of **2** DECRAs, **5** ARC Linkage Projects, **4** ARC Discovery Projects and **1** ARC Industrial Transformation Training Centre
- **More than 300** technical journal articles.
- Connections with **more than 50** overseas universities.
- **More than 40** industry partners.
- Industrial test-beds at various scales

In addition, the BIM Centre has a strategic alliance relationship with the Sustainable Built Environment National Research Centre (SBEnrc). The SBEnrc is the successor to CRC on Construction Innovation. Established in 2010, SBEnrc is a key research broker between industry,

government and research organisations for the built environment industry. The SBEnrc has focus on the areas that will deliver improved sustainability outcomes for built environment and the Australian community, especially through increased uptake of innovative practices. Both centres have established strong relationship with road stakeholders, including NSW RMS, QTMR and MRWA demonstrated by prior engagement and collaborative research projects.

Professional activities

He is on the Board of Directors and country representatives of International Society of Computing in Civil and Building Engineering (ISCCBE) and International Association of Automation and Robotics in Construction (IAARC), two most highly regarded academic societies in Automation in Construction. He was the editorial board member for ASCE Journal of Construction Engineering and Management for numerous years and Journal of Information Technology in Construction. He is the editor/co-editor of four conference proceedings and the guest editor of Journal of Automation in Construction", "Journal of Information Technology in Construction", on various topics in Construction Engineering and Management. He chaired three international conferences specialized in the area of Construction IT and is chairing the Global Lean Construction Conference 2015. He is the Editor-in-Chief of Springer Journal "Visualization in Engineering". He is currently the principal supervisor to 14 post-doctoral fellows and 25 full time Ph.D. students.)

Leaderships

He solely founded a Research Centre at Curtin from 1 person to almost 50-researcher during past four years with near to USD $ 20 million across 80 projects. The Centre is highly interdisciplinary and closely works with industry. Prof Wang established and led a reputable industry-focused collaborative research alliance that strives to improve productivity in LNG construction and maintenance by synergizing theory with practice. Impact of his work is highlighted by his establishment and leadership of a reputable industry alliance where over 40 industry partners are significantly contributing. The alliance is well positioned to lead the research, innovation, and industry practices towards improved productivity in World's energy industry.

Prof. Wang has completed a number of research projects related to smart sensing. Because of his research contribution, he has been invited to give **more than 50 keynote presentations** in international conferences and **over 80 public talks** in government, companies, and universities/schools on a wide range of topics. His presentations topics are related to construction informatics, Building Information modelling and virtual reality. He has chaired and organized **over 20 events** including several prestigious international conference, such as the 23rd Global Lean Construction Conference (ERA Ranking – A) which has **over 500 attendees** and half of them were from industry. His professional leadership and activities are highlighted by that he sits on chair or session chair committee of **over 30 events**. He is also the members of **over 70 scientific committees** for international events. He is the founder and editor-in-chief Journal of Visualization in Engineering, and also serves on board for **over 10 journals** and reviewers for **40 journals** across various engineering and technology disciplines. The publications of Prof. Wang have attracted **close to 6,000 citations** in Google scholar with an H-index of about **40**. These numbers are extraordinarily high for the discipline of civil engineering. Prof. Wang's name and research work has been cited in The International Directory of Experts and Expertise, Who's Who in Engineering, Who's Who in Fine Arts, etc.

Representatives Research Projects

In the last six years, Prof. Xiangyu Wang has secured more than USD $20 million funding from the industry and the commonwealth government, demonstrating his research impact. Some of the most notable projects include:

- ARC Linkage Project, LP180100222 (2019-2021): "Asset intelligence: Maximising operational effectiveness for digital era", awarded amount: $ 436,824
- ARC Discovery Project, DP170104613 (2017-2019): "Automatic construction monitoring through semantic information modelling", awarded amount: $547,500
- ARC Discovery Project, DP170104612 (2017-2019): "A multi-agent system for stakeholder management in off-site construction", awarded amount: $432,000
- Australian Research Council (ARC) Linkage Grant (LP160100528) (2016-2019): "Bridge Performance Assessment through Advanced Sensing and Modelling", awarded amount $280,000
- Sustainable Built Environment national research centre (2017-18): "Developing a Cross Sector Digital Asset Information Model Framework for Asset Management BIM Information Modelling" awarded amount $270,132
- Huawei Technologies Co. Ltd., Main Roads Western Australia, NSW Roads and Maritime Services, Aurecon (2016-2019): "Bridge Performance Assessment through Advanced Sensing and Modelling", awarded amount $170,000 (Industry cash contributing to ARC Linkage LP160100528)
- UGL Inc. (2016-2018): "Lean LNG Plant shutdown: under the Principles of Curtin's Advanced Technologies Research and Innovation Alliance (CATRINA)" awarded cash amount $300,000; in kind amount: $300,000
- Woodside (2016-2018): "Lean Maintenance Research to minimize shutdown turnaround time: under the Principles of Curtin's Advanced Technologies Research and Innovation Alliance (CATRINA)" awarded cash amount $150,000; in kind amount: $150,000
- Kaefer (2016-2018): "Digital Scaffolding to Reduce Costs: under the Principles of Curtin's Advanced Technologies Research and Innovation Alliance (CATRINA)" awarded cash amount $160,000
- Shell Inc. (2016-2018): "Container Insert, Mercury Disposal and FLNG Logistics Studies under the Principles of Curtin's Advanced Technologies Research and Innovation Alliance (CATRINA)" awarded amount $300,000
- Australia-Korea Foundation, Department of Australian Foreign Affairs and Trade (2015-2016). "Australia-Korea Forum for Offshore Technology in Oil & Gas Industries (AKO 2015)." awarded amount $20,000
- Australian Research Council (ARC) Linkage Grant (2014-2017): "Boosting Up Productivity: Optimising Scaffolding Life Cycle Management through Virtual Design and Construction", awarded amount $427,500
- Australian Research Council (ARC) Linkage Grant (2013-2016): "Transforming liquefied natural gas (LNG) plant construction productivity through mobile computing technologies", awarded amount $500,000
- Sustainable Built Environment National Research Centre with Woodside Energy Ltd., John Holland Inc., Main Roads Western Australia, Queensland Transport and Main Roads (2014-2017): "Boosting Up Productivity: Optimising Scaffolding Life Cycle Management through Virtual Design and Construction", awarded amount $250,000; (Industry cash contributing to ARC Linkage)

RESEARCH IMPACT

Prof. Wang had made distinctive contributions in BIM applications in the real world. He has undertaken a number of real world BIM application projects with Woodside Energy Ltd., Prof. Wang used the combination of onsite tracking and sensing with in-house and onsite visualization to quickly capture human errors in procurement, materials tracking, construction process control and monitoring, and commissioning and operation. This has significantly reduced the amount of rework, resulting in significant cost saving. Those projects have successfully scaffolded the research team led by Prof Wang to win an ARC LP funding commencing from 2013 to significantly bring those initiatives into the future stages (ARC LP130100451).

Professor Wang's work has been reported by **over 30 times** by various national and international Medias. Some examples can be found in:

- The "Australian" Newspaper in 11th September 2012
- The "Australian" Newspaper, in 20th May, 2014
- LNG World News titled "Woodside: Pioneering Visualization Technology Research"
- Business News WA, 22nd Sep., 2014

Prof. Wang has attracted and led over 40 industry-funded research projects in the past five years across four sectors: oil and gas, mining, infrastructure, and building.

- In the **oil and gas sector**, Project Echo is Woodside initiated project with over 30 industries involved. His significant research on Project Echo is to investigate a suite of new technologies, approaches, and concepts in improving the productivity, performance, and safety along the life cycle of any built asset in the oil and gas industry that includes onshore LNG plant, offshore LNG facility, and floating systems.
- In the **mining sector**, he has developed a novel approach to integrate BIM and optimization together to generate maintenance schedules for plant shutdown. The results show that this method can reduce direct cost significantly.
- In the **infrastructure sector**, Prof Wang has led a couple of significant research projects funded by two Government bodies: Western Australian Main Roads and Queensland Transport and Main Roads. He also led the development of National BIM Guidelines for Australian Infrastructure.
- In the **building sector**, Prof Wang has entered an agreement with BPI to extensively study how the site productivity can be improved on the Westin Hotel project, located in 480 Hay Street in Perth CBD. Prof Wang's outstanding high industry impact work with Australian Industry have been reported by international and domestic media for over 20 times, including twice by The Australian Newspapers.

Some specific examples which can demonstrate Prof. Wang's research impact in the discipline include: Prof Wang has worked with Woodside in the oil and gas sector to introduce the LNG Smart Tag System ("Woodside tags a smart savings idea", The Australian Newspaper, 2014.) that could identify and locate site materials in 3D in real time (https://www.youtube.com/watch?v=ztILo5FHt54). The system has cut wasteful downtime by ensuring that the millions of parts that go into constructing and maintaining an LNG plant are quickly identified, located and retrieved. The smart tags have been launched at the Woodside operated Plant and operators from Europe, Asian, North and South America have expressed strong interest in the trials ("LNG Smart Tag", 2014, WA:ERA News). He also works closely with a few SME to improve their business through innovation and technology uptakes. For example, his work with Saleen Technologies Inc, led to the solutions to tracking construction parts by combining Slaeen's barcode technologies in a very unique way with GPS, and the Woodside Smart Tag. The work has proved to save money: a quote from one unnamed client informed that the system had saved the company $ 1.4 million in a few months (Energy Publications "Woodside on board Track'em's trail" featured Prof. Wang's photo).

Dynamic Flexoelectric Effect on Piezoelectric Nanostructures

by Timon Rabczuk, Member EUAS

Short Biography

Prof. Dr.-Ing. at Bauhaus University Weimar, Chair of Computational Mechanics
Former Director of the Institute of Structural Mechanics, Bauhaus University Weimar
National High End Foreign Expert at Tongji University, Shanghai, China
More than 200 SCI publications
Listed in ISI Highly Cited 2014 and 2015 in 'Computer Science' and 'Engineering'
ERC-CoG COMBAT
Coordinator of ITN-INSIST and IRSES-MULTIFRAC
Prof. Rabczuk is Full Professor at Bauhaus University Weimar and listed as highly cited researcher of Thomson Reuters/Clarivate Analytics in Computer Science and Engineering since 2014 (until now). The research focus of Prof. Rabczuk is Computational Solid Mechanics with emphasis on method development for problems involving fracture and failure of solids and fluid-structure interaction. He is currently developing deep energy methods and machine learning based approaches for the solution of PDEs, nonlocal operator methods and formulations based on Isogeometric Analysis. Another key research direction is Integrated Computational Material Engineering/Computational Materials Design with focus on polymer-matrix composites, batteries and recently phononic topological insulators.

Dynamic Flexoelectric Effect on Piezoelectric Nanostructures

B.H. Nguyen, S.S. Nanthakumar, X. Zhuang, P. Wriggers, X. Jiang, T. Rabczuk

European Journal of Mechanics / A Solids 71 (2018), 404-409

Abstract

Flexoelectricity, which represents the spontaneous electric polarization induced by the strain gradient, is a universal electromechanical coupling effect regardless of symmetry in all dielectric material. In solid dielectric material, the contribution from flexoelectricity can be due to four related phenomena: static and dynamic bulk flexoelectricity, surface flexoelectricity and surface piezoelectricity. While the surface flexoelectric effect can be negligible, the magnitude of the remaining three phenomena are comparable. Presently, the role of the static bulk flexoelectric and surface piezoelectric effects in the energy

harvesters has been intensively studied, the contribution from dynamic flexoelectric effect remains unclear. In this work, based on the conventional beam theory, equations of motion considering dynamic flexoelectric effect are investigated. Consequently, the free vibration of the simply supported beam is studied in order to examine the influence of the dynamic flexoelectricity on natural frequency. From the numerical studies, it is found that dynamic flexoelectric effect is more influential on thick beam model and higher vibration modes. In addition, the results show that the relation between the static and dynamic flexoelectric coefficients can also alter the free vibration response.

Numerical Model for the Characterization of Maxwell-Wagner Relaxation in Piezoelectric and Flexoelectric Composite Material

B. H. Nguyen, X. Zhuang, T. Rabczuk

Computers and Structures 208 (2018) 75–91

Abstract

Bi-layer structures can be engineered to investigate the interfacial polarization (Maxwell-Wagner polarization) of heterogeneous dielectric material, which shows the frequency-dependent property of the effective dielectric permittivity. However, in piezoelectric or flexoelectric heterostructures, behaviors of the effective piezoelectric or flexoelectric coefficients are remained unclear. Therefore, in this work, we present a numerical model of the Maxwell-Wagner polarization effect in a bi-layer structure made of piezoelectric or flexoelectric material. In this model, the conductivity, which qualitatively represents the free charge in a real dielectric material, is introduced to the complex dielectric permittivity.

Several numerical examples are performed to validate the model and investigate the frequency dependence of the effective dielectric permittivity, piezoelectric and flexoelectric coefficients as well as the giant enhancement of dielectric constants. It is found that the static (at low frequency) and the instantaneous (at high frequency) effective coefficients are governed by those of the thin and thick layer, respectively. Moreover, both conductivity and volume ratio play essential roles in the enhancement of the dielectric constant that is underpinned by the Maxwell-Wagner effect.

A Large Deformation Isogeometric Approach for Flexoelectricity and Soft Materials

Tran Quoc Thai, Timon Rabczuk, Xiaoying Zhuang

Comput. Methods Appl. Mech. Engrg. 341 (2018) 718–739

Abstract

We propose an isogeometric approach for flexoelectricity in soft dielectric materials at finite deformations accounting for Maxwell stresses on the surface between two different media. In contrast to piezoelectricity where there is a linear dependence between mechanical strain and electric polarization, in flexoelectricity the polarization is related to strain gradients which requires a C^1 continuous finite element framework. In electro-mechanical materials, the Maxwell stress emerges as a consequence of the coupling effect between electrostatics and mechanics. If a solid body is embedded in a surrounding medium such as air or vacuum, the Maxwell stress acting on the surfaces governs the interaction between electric fields and deformable media. This is quite difficult to handle due to the surface discontinuity and the traction electrical forces still have to satisfy some certain continuity conditions, hence an appropriate numerical framework is required for the treatment. Here, we employed Non-Uniform Rational B-spline (NURBS) functions with knot insertion technique in order to introduce discontinuities across material interfaces while still maintaining C^1 continuity in the domain to evaluate the coupling effect of strain gradient and electric polarization in the regime of finite deformation. The accuracy and robustness of our IGA approach for flexoelectric soft materials are demonstrated in some benchmark numerical examples.

Robotics for Societal Services

by Aarne Halme, Member EUAS

Short Biography

Aarne Halme is emeritus professor of Aalto University (before Helsinki University of Technology), Finland, and Chairman of the Board of GIM Ltd. His background is in control and systems engineering. He started academic carrier in 1972 as an associate professor of control engineering at Tampere University of Technology. In 1977 he moved to Oulu University, where he was professor of control and systems engineering. From 1986 until retirement he has been professor of automation technology at Helsinki University of Technology, where the period 2008-2013 he was the head of the Academy of Finland Centre of Excellence in Generic Intelligent Machines. After retirement 2014 he established with his colleagues GIM Robotics company (www.gimltd.fi), which continues the activities of the Excellence Centre on commercial bases. He has made both theoretical and practical research in many fields of systems science and automation. Since mid 80's he has worked actively with intelligent field and service robotics research including development of mobility means, like walking and hybrid mechanisms, navigation and perception systems, and interactive human robot interfaces. His scientific interest includes also new energy technologies especially fuel cell systems intended to use in mobile devices. Publishing includes more than 200 articles in scientific journals, conference and books

My interest in robotics is in the field and service robotics. This genre of robots comprises robotic machines that work outside factories replacing people in tasks, which are monotonous, dangerous or do not any more fulfill the minimum requirements for human work. The robots operate often in an environment unfriendly for humans or offer help or entertainment services to people in their homes and public places. Task scenario usually includes an environment, which is not well structured, not a priori known in details and may be changing with time. Often high autonomy is needed. Such environments are typical also for biological species that often act as models for engineering designing. In most cases robots must be mobile, because tasks cannot be moved to the robots (like in factories), but robots must move to the tasks. Research and development of field and service robots has been active since mid 80s and we have seen many interesting robots in media.. It is important to note that appearance of those robots may vary a lot depending on their application field, size and tasks they are intended. Human like robots are rather exceptions than the rule. Many field robots are designed by automating existing work machines. In the figure below some of those robots are visualized.

In field robotics applications vary from farming, construction and utilization of natural resources like mining, to exploration of planetary system (moon, planets, asteroids). Important application area is also undersea operations, where robots replace people in deep waters. **In service robotics** home services, entertainment, disabled support, replacing manpower in human-intensive non-industrial work in offices, hospitals, public places, hostile urban environment (cleaning streets, sewers etc) are the main application areas. Outside normal civil tasks military technology, rescue operations and catastrophe aftercare use increasingly robots today.

There are two main challenging technological steps in modern robotics in its way from factories to among people. The first to be taken is to obtain fluent mobility in unstructured, changing environment, and the second is to obtain the capability for intelligent communication with humans together with a fast, effective learning/adaptation to new work tasks. The first step has almost been taken today. The rapid development of sensor technology – especially inertial sensors and laser scanners – with constantly increasing processing power, which allows heavy image processing and techniques for simultaneous localization and mapping (SLAM), have made it possible to allow slowly moving robots to enter in the same areas with humans. However, if we compare the present capability of robots to animals, like our pets in homes, it can be said without no doubt that improvements are still possible and desirable. The second step is still far away. Traditional industrial robots are mechanically capable to change a tool and perform different work tasks, but due to the nature of factory work need for reprogramming is relatively minor and therefore interactive communication with the user and continuous learning are not needed. The most sophisticated programming methods allow task design, testing, and programming off-line in a simulation tool without any contact to the robot itself. Today's commercial mobile service robots, like vacuum cleaners and lawn mowers, are limited to a single task by their mechanical construction. A multi-task service robot needs both mechanical flexibility and a high level of "intelligence" in order to carry out and learn several different tasks in continuous interaction with the user. Instead of being a "multi-tool" the robot should be capable of using different kinds of tools designed for humans. Due to fast development in mechatronics, hardware is not any more the main problem although the prices can be high. The bottlenecks are the human – robot interface (HRI) and the robot intelligence, which are strongly limiting both the information transfer from the user to the robot as well as the learning of new tasks.

Despite huge efforts in Artificial Intelligence (AI) and robotics research, the word "intelligence" has to be written today in quotes. Researchers have not been able to either

model or imitate the complex functions of human brains or the human communication, thus today's robots hardly have either the creativity or the capacity to think. The main requirement for a service robot HRI is to provide easy humanlike interaction, which on the one hand does not load the user too much and on the other hand is effective in the sense that the robot can be kept in useful work as much as possible. Note that learning of service robots new tasks is not counted as useful work! The interface should be natural for human cognition and based on speech and gestures in communication. Because the robot cognition and learning capabilities are still very limited the interface should be optimized between these limits by dividing the cognitive tasks between the human brains and robot "intelligence" in an appropriate way. The answer is to use multi-modalities i.e use all communication means natural to human to communicate the task to the robot. This means using audio-visual means together with traditional IT-communication means. The picture below illustrates a robot, called WorkPartner, and a task (cleaning snow from yard) we have used to research different means to communicate the task effectively on-line to the robot. In this case we utilize human cognition and common spatial awareness of the robot and the human. The key component in communication is a sign showing position and direction which the robot can read by camera vision. The software recognize the task details and control the robot after the human has marked off the area to be cleaned and gives voice commands define the details of the work (like where to heap the snow). By this way we avoid the time consuming use of map based configuring of the task which is be the traditional way doing it.

More details on this topic and the story of WorkPartner robot, which is one of the world's most advanced service robot, can be found from articles listed references. More information and videos can be found under the link http://autsys.aalto.fi/en/WorkPartner.
During last ten- fifteen years there has been growing interest to use robotics in **societal services** to support activities like senior citizens living in their homes, disabled persons mobility, guarding and security in public places, only to mention a few. Basically the tendency is to increase the level of automation but in a way that fits to peoples living environment. In all these applications the human user is very close to the robot and the meaning of the interface is crucial in successful cooperation. In many cases it is useful to use multi-modalities in communication, i.e. speech, haptics and gestures in addition to traditional keyboard type of interfaces. It is also important to balance the human decisive actions with the robot own "intelligence". In addition to avoid unwelcome development in artificial intelligence we can often reduce significantly size of the robot software. This in turn means usually increasing reliability and decreasing price of the robot as a product.

Currently my interest in this genre of robots is focused to developing a guide robot for visually impaired. It is a robot that functions like today's trained guide dogs providing the guiding services when blind people move outdoors on their trained routes. Why a guide robot? Based on WHO statistics (2012) there are 314 million of visually impaired in the world who need assistive products to manage their everyday life. In Finland alone, where I live, there are about 80 000 of which 10 000 employed and 70 000 outside employment. There are numerous assistive technologies to compensate low visual performance with other senses, especially with sense of touch. Guide dog is meant to support the visually impaired to move outside his/her home. Guide dog supports the user to avoid obstacles, to cross the street and to avoid rough surfaces etc.

A guide dog helps the user to find
a passable path by pulling with slight force.

Guide dogs are specially trained, selected dogs and their training and administration is expensive. With modern robotics it is possible to replace the guide dog and offer all the supportive features a guide dog can offer. A dog is also a pet, the robot can't and should not compete in this role. On the other hand, a robot as a technical device does not commit the user in the same way as a dog. The benefits of robot technology are economy, easy duplicating, precision with modern sensor technology and many additional services that can be built into the system.

Guide robot development benefits recent progress in sensor technology. Lidar (light detection and ranging) sensors and cameras offer economic solution to detect environment geometry with high precision. Ultrasound and RF technology can give additional information. Reliable localization and navigation both indoors and outdoors can be based on several methods utilizing available radio beacon signals and perceived environment information. With these technologies combined a guide robot can have a sensing system that warns about obstacles and can guide visually impaired through a safe route. The robot will move on the side of a person or little ahead and has weak pulling effect like a guide dog. Move on wheels gives feeling of surface forms to the user of the robot. Modern accurate navigation system and digital maps offer additional features to the robot like automatic navigation and using a route predefined on the map – these features do not exist having a guide dog. Continuous 3D mapping of the environment can create innovations improving the support a robot can give to the visually impaired.

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Low CO2 Emission Power Generation System Utilizing Oceanic Methane Hydrate

by Shigenao Maruyama, Member EUAS

Short Biography

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Academic Qualifications

B.Eng. 1977, Department of Mechanical Engineering II, Tohoku University, Japan
M.Sc. 1979, Department of Aeronautics, Imperial College, London University, UK
M.Eng. 1980, Department of Mechanical Engineering, Tohoku University, Japan
PhD 1983, Department of Mechanical Engineering, Tohoku University, Japan

Professional Carriers

1983 Assistant Professor, Institute of High Speed Mechanics, Tohoku University
1988 Visiting Scholar, School of Mechanical Engineering, Purdue University, USA
1989 Associate Professor, Institute of Fluid Science, Tohoku University
1997 Professor, Institute of Fluid Science, Tohoku University.
2005-2006 Specially Appointed Assistant to the President, Tohoku University
2006-2009 Councilor, Tohoku University
2006-2008 Special Advisor to President, Tohoku University
2006-2013 ***Special Advisor for Centenary Events and Alumni, Tohoku University***
2008-2011, 2015-2017 Distinguished Professor of Tohoku University
2016 Visiting Professor, INSA de Lyon
2017- President, National Institute of Technology, Hachinohe College

Awards

Japan Society of Mechanical Engineers (JSME), Award for Young Engineers, 1989
Fluid Science Foundation, Award for Fluid Science, 1995
Heat Transfer Society of Japan (HTSJ), Award for Scientific Contribution, 1998, 2016
JSME Medal for Outstanding Paper, 1999, 2013
HTSJ, Award for Scientific Measurement, 1999
JSME Tohoku Division, Award for Technical Contribution, 2001
Japan Society of Applied Electromagnetic and Mechanics, Best Technical Contribution Award, 2001
JSME Thermal Engineering Division, Award for Academic Achievements, 2001
HTSJ, Award for Technical Contribution, 2002
Societe Francaise de Themique, 2002 International SFT Award, 2002
JSME Thermal Engineering Division, Award for Contribution, 2003
JSME Fellow, 2004
Government of Japan, Japanese Medal of Honor (Medal with Purple Ribbon), 2012
JSME Thermal Engineering Division, Award for Achievements (Research), 2012

Research Activities

Professor Shigenao Maruyama specializes in thermal engineering. He has published more than 10 books and 200 academic research papers, and has acquired 50 patents. He investigated various aspects of fluid flow and energy exchange. Based on the principle that conventional heat transfer and thermal control focuses on the enhancement of heat transfer and temperature control of equipment, he has proposed a novel concept of heat-transfer control, in which the heat transfer is actively enhanced or reduced. The proposed active thermal insulation system and a heat-transfer control device utilizes Peltier effects. His work is interdisciplinary utilizing knowledge from various academic disciplines. He has co-authored and edited Thermodynamics (JSME Text series) [1], one of the bestselling books on thermodynamics for mechanical engineering students in Japan. He has also published a book to educate the public thermal science [2], and a

novel describing accidents in Fukushima Daiichi nuclear plants [3].
Some aspects of his research activities are as follows:
Radiative heat transfer: *Detailed studies on radiative heat transfer, which is energy transfer by infrared or electromagnetic waves, has been carried out. A generalized analysis method to calculate radiative heat transfer was proposed [4], and this method was applied to analyze heat transfer in semi-conductor processes [5] and industrial furnaces. This method was also applied to large-scale environmental energy transfer processes, such as heat transfer in fogs and clouds [6]. Thermal emission from nano-scale structures was also investigated [7]. These results were published in a monograph [8] which is the first textbook on radiative heat transfer in Japan.*
Natural convection: *Natural convection induced by temperature differences in fluid and the gravitational force was studied, and a generalized description was presented [9]. These results were applied to the cooling fins of electronic devices [10]. This research has been extended to understanding large-scale natural convection in oceanography. The up-welling velocity of deep seawater in the ocean which was proposed by Stommel to be a perpetual salt fountain, was successfully measured for the first time in the world [11].*
Active heat-transfer control by Peltier elements: *Peltier elements, used as cooling equipment, have been applied to a heat-transfer control device. This device has been utilized to the heat-transfer control of equipment in a microgravity environment [12], in an active catheter, and in artificial heart muscles [13]. Furthermore, this heat-transfer control has been applied to the fields of oriental medicine and cryosurgery [14]. The concept of heat-transfer control has been expanded to fusion of thermal engineering and medical engineering [15].*

Introduction

Global warming is one of the most important issues that humankind is facing today. The concentration of carbon dioxide (CO_2) in the atmosphere was 280 ppm in the 14th century and had been stable until the 18th century. The advent of the Industrial Revolution at the end of the 18th century brought about an increase in the CO_2 concentration in the atmosphere, and by 2015 this concentration had exceeded 400 ppm. The Intergovernmental Panel on Climate Change (IPCC) pointed out that the global warming in turn has led to an increase in climate change related events such as natural disasters.

The total amount of CO_2 emission in the world is increasing every year in spite of technology development for high efficiency power generation systems. One of the solutions to reduce the CO_2 emission could be CCS (Carbon Capture and Storage) technology. We proposed a low CO_2 emission power plant combined with an Oxy-fuel combustion process and a CCS system [16].

Methane hydrate (MH) is a new type of energy resource. MH generally exists in the solid state with molecular methane caged inside molecular water crystals, and is being widely mined under the oceans. It is estimated that the hydrate mine in the Nankai Trough, Japan, can provide a stable energy supply that will meet more than ten years of Japan's natural gas demands, which is very promising, especially for a country with highly dependent on energy imports.

The world's first oceanic methane hydrate production test was conducted in 2013 in the Nankai Trough. More recently in 2017, a new production test was conducted there. Nearly the same period, the first extraction operation in China was carried out in the Shenhu area of the South China Sea. Such developments demonstrate the real feasibility of using MH for domestic or industrial purposes in the near future, even though there are many problems to be resolved towards an economical production target.

Proposal for a low CO_2 emission power generation system utilizing oceanic methane hydrate (MH)

We proposed a power generation system with low carbon dioxide (CO_2) emission [17], as shown in Fig. 1. This system simultaneously carries out power generation, MH

utilization, and carbon dioxide capture and storage (CCS). In this system, CO_2 resulting from the combustion is dissolved in seawater. A thermal stimulation method was selected to dissociate the oceanic MH. CO_2-dissolved seawater is heated by the high-temperature exhausted gas from power generator and injected into the hydrate layer to dissociate the methane hydrate. A feasibility study of the proposed system using process simulations showed that a power generation system with approximately 30% thermal efficiency and above 90% CO_2 recovery rate was achieved.

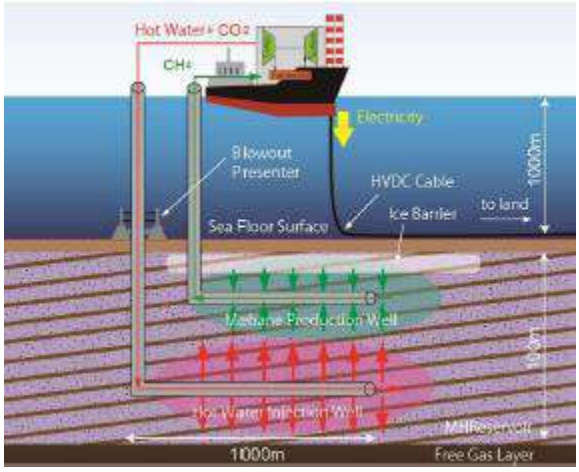

Fig. 1 Concept of an oceanic MH power generation system with a concurrent CCS process.

According to the system simulation of the MH power generation system, the increase in production rate of methane gas is the key to an economically feasible plant. Further, the likelihood of constructing the economically feasible MH plant would be greater if the electrical energy produced was sold at the price of renewable energy.

We also proposed a batch type design facilitated with a vertical production well system and a warm-up process, as shown in Fig. 2, which is executed before and during the continuous gas extraction process from the MH reservoir [18]. The system includes a methane gas production well using depressurization, a hot water/CO_2 re-injection well, and a power generation system. The re-injection of hot water/CO_2 sustains the sensitive heat required for the dissociation and extraction processes in a strategic production lifecycle.

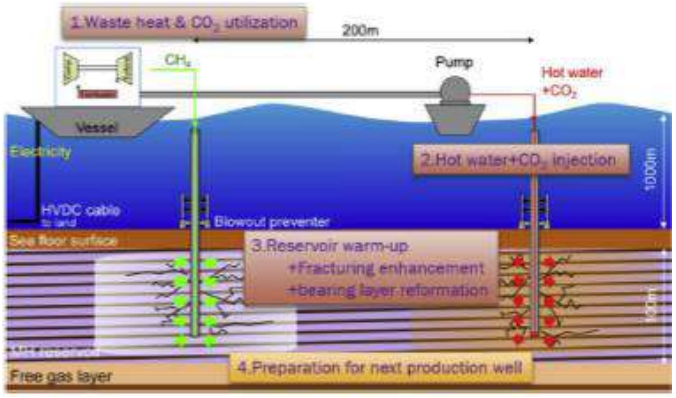

Fig. 2 MH power generation system using strategic warm-up process, along with CCS and vertical wells.

Numerical simulations show that this design has the potential to enhance long-term gas production. Thermal balance and sensitive heat supply are of special importance for the production rate. The analysis of the power generation and CCS systems in this design show a general efficiency of 40%. The selection of amine for CO_2 separation, the effect of injection conditions of hot water/CO_2 and the feasibility of the proposed methane extraction and power generation system were also discussed in detail.

Measurement of MH dissociation and core size experiment

In order to construct a numerical model of the reservoir-scale production, a very precise in-situ measurement system to measure the dissociation process of MH was constructed [19]. This system is a Mach-Zehnder interferometer. This interferometer is approximately 100 times more accurate than a conventional interferometer, by utilizing the phase-shifting technology. High-speed measurements can be achieved by introducing the newly developed arbaa prism.

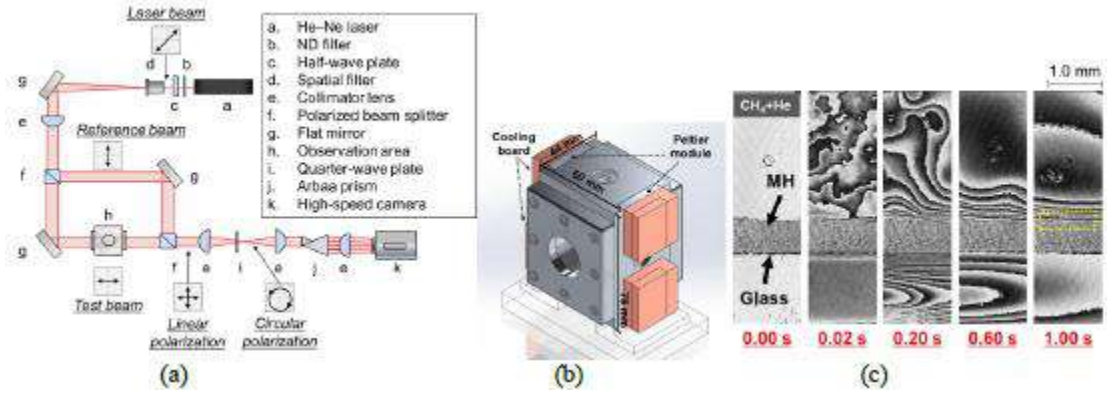

Fig. 3 High-speed phase-shifting interferometer (a), test cell for MH dissociation (b), and in-situ phase-shifting interferograms at MH dissociation (c).

The transient variation of density field and the dissociation of MH near the interface were measured using the measurement system [20]. The dissociation rate estimated from the experiment was compared to the numerical simulation. Experiments were conducted in a core-sized container with a mixture of sand and synthesized MH [21]. The results were compared to a numerical simulation developed for a large scale MH mine.

Construction and simulation of reservoir scale model for production and utilization of methane hydrate

This study focuses on the utilization of oceanic MH as an energy resource under the real production situations. We discussed the developments associate with MH production and major challenges foreseen from the reservoir-scale analysis. A numerical model was developed based on the geological conditions of the Nankai Trough. The effects of boundary conditions and reservoir parameter on the production rates are discussed in detail [22]. Furthermore, we found that the injection of hot water into the MH mine increases the temperature enhancing the production rate substantially. The cracks in the mine produced by injecting high-pressure and high-temperature sea-water enhances the heating of the mine, and the production rate of methane gas is much increased. This high production rate is the key parameter for the commercialization of the MH power plant.

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The Science of Human - Machine Systems

by Peter Hancock, Member EUAS

Short Biography

Peter Hancock is Provost Distinguished Research Professor at the University of Central Florida. He has been awarded the Sir Frederic Bartlett Medal of the Ergonomics Society of Great Britain, the Liberty Mutual Medal of the International Ergonomics Association, and the Jastrzebowski Medal of the Polish Ergonomics Society and has been continuously funded by extramural grants every year of his professional career. His current experimental work concerns time and behavioral response in high-stress conditions. His theoretical works concerns human relations with technology and the future of this symbiosis. He is a Fellow of, and past President of, the Human Factors and Ergonomics Society.

Preamble

This brief synopsis serves to introduce myself and the branches and tranches of science that I pursue. It is not an exhaustive exposition but rather focuses upon the concerns of human-technology interaction which form perhaps the largest focus area of my endeavors. I look to show how this concern for human-technology interaction is central to other aspects of the research in which I engage.

The Sciences of Human-Machine Systems

I think it is reasonable to assume that technology is the most powerful tool humans have created, so as to be able to fashion and shape the world around them. I also think it is fair to observe that such technologies are not flawless, nor do they always work in ways that can be readily anticipated and predicted. Some would argue that these are actually necessary shortfalls that accompany highly complex systems, operating in evidently uncertain environments. Thus, guarantees and imprimaturs of success can only be assured within certain reasonably specified bounds. Each of us can attest to the public furor when any of these large-scale systems fail in any manner. Indeed, the names of these failures: *Deep Water Horizon, Piper Alpha, Challenger, Herald of Free Enterprise, Fukushima, Columbia*, etc. resonate across all of modern Society. The area of science within which I primarily work, is variously called *Human Factors*, *Ergonomics*, *Human-Engineering*, and *Human-Systems Integration*. This branch of science searches for both reactive and proactive insights into such complex systems operations in order to both prevent disaster and foster operational success. The systems so studied can range in scale and extent from a single hand-held tool to global computational systems. Our science (from here on referred to as *Human Factors/Ergonomics [HF/E]*) seeks to distill and apply principles which extend across such vast ranges and time-scales of action. HF/E is, at the moment, most especially concerned with human interaction with ever-more autonomous systems; paradoxical though such a statement might appear. It is from the well-spring of such counter-intuitive observations and asservations that the great value of HF/E emerges.

An Origin in Conflict and Disaster

Although the study of human beings at work goes back some centuries (Ramazzini, 1713; Jastrzębowski, 1857), the great impetus for understanding how people operated with, and sometimes failed with, technology was impelled largely by the exigencies of World War II. Some of the pragmatic origins of HF/E go back to the crucial observations of those such as Vannevar Bush (1945) who understood that those who best utilized technological advances in support of their various forces would prevail in that and following conflicts (and see Licklider, 1960). Yet, and it is sad to say, HF/E often finds itself the beneficiary of the aforesaid large-scale disasters. One such pivotal event in the United States was the incident at *Three-Mile Island* (Perrow, 1984). At the time of this incident, I was a graduate student. However, like many others, I felt the impact on the discipline I had chosen to follow, even from such a lowly position.

As with the early work on issues such as pilot error during the Second World war, it had been traditional to follow the easiest path of causation and blame the one single, fallible human (who now, rather fortunately, was mostly not around to dispute the issue) (cf., Wilder, 1927). This 'human error' approach had provided a comforting pabulum, especially when compared to the acknowledgement of rather more systematic source of failure. Our HF/E heroes (e.g., Chapanis, 1965, Fitts & Jones, 1947) eschewed this highly simplistic interpretation, especially as a wide-range of varied individuals all seemed to be making exactly the same mistake. The real birth of HF/E came with the recognition that there were system-induced errors, inadvertently designed into complex systems, which caught out fallible humans over and over again. When the '*blame the user'* fallacy was fully exposed, HF/E, as a branch of science, took off. It has been battling such simplistic interpretations of complex human-machine behaviors ever since.

My Life in Human-Machine Systems Science

My entry in HF/E was idiosyncratic. It turns out that this is not uncommon in that many in HF/E come from highly diverse backgrounds, emerging from studies in disciplines as diverse as, philosophy, art, design, psychology, mathematics, engineering, biology, and the neurosciences, in addition to a host of others. I shall not rehearse my own particular autobiographical path here, since that story is already published and readily available (Hancock, 2012). Rather, what I would like to do here is expand upon my current pursuits and concerns. My Laboratory works, at this time, on experimental studies concerning human-robot interactions (see e.g., Hancock et al., 2011; Kaplan et al., 2018; Sanders et al., 2019; Volante et al., 2019). Most particularly, we are concerned with the issue of trust, which features heavily in the Lab's experimental program (Hancock, Billings, & Oleson, 2011; Phillips et al., 2016). Most recently, this has expanded to include work on the usability of robots by the disabled (Sanders et al., 2017). At one and the same time, we have been examining other facets of subjective response to technology, and here the concerns for mental (cognitive) workload evaluation have come to the fore (Hancock, 2017; Hancock & Matthews, 2019; Matthews, De Winter & Hancock, 2019). Considerations for cognitive workload has been a consistent thread in my research, now across multiple decades (Hancock & Meshkati, 1988; Hancock, Meshkati, & Robertson, 1985). The focus on robots has also expanded to include many sorts of automation in general (Schaefer et al., 2016). Within most recent months this has also been elaborated into a focus on automated vehicles (Hancock, 2019a; Hancock, Nourbakhsh, & Stewart, 2019). This has echoed a long-standing concern in my career for road safety and driver

performance (Hancock, Wulf, Thom, & Fassnacht, 1990).

While each of the projects or programs I have pursued tend to feature a particular expression of technology, it is the wide swath of progress which is always informing and directing my research. I have been especially interested in the way in which technology acts as a conduit to express society's purposes in life (Hancock, 2009). Here, I have been troubled by the ways in which much of technological development appears to happen in the relative 'vacuum' of the market and its forces, rather than emerging from a more informed and intentive discourse. Recently, I have had the opportunity to revisit a chapter I published now some quarter of a century ago (Hancock, 1996). In the associated commentary (Hancock, 2019b), I have lamented that disturbingly little progress seems to have been made in respect of 'mindful' design and developments in technology in the interim period. This lamentable lack of progress is set against a background of, what I have termed, incipient *civicide* (Hancock, 2019c). While HF/E aspires to, and embraces the goal of, adding to the quality of human life, the pertinent question that remains largely unanswered is whose specific life we are looking to improve here. I hope to be allowed sufficient time in life to see that expression extend to all human beings on our planet; yet, the putative 'progress' of our times seems rather to militate against any such achievement. As a working scientist, I am motivated each day to try to improve our collective existence. As an observer of our current world, I am left in doubt about the rationality of that course of action.

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Time-Dependent Reliability of Engineering Structures

by Guiqing Li, Member EUAS

Short Biography

Prof. Li graduated from civil engineering department of Hunan University of China in 1953. He was a postgraduate student studied structural dynamics in Harbin University of Technology in the period from 1959 to 1963. He was a Director, International Association of Structural Reliability and Safety; Director, China Association for Disaster Prevention; Vice Chairman, Council of Wuhan University of Technology (WUT); Vice Chairman, Society of Sciences and Technology, WUT; Vice Chairman, Academic Committee, WUT; Director, Institute of Aseismic Engineering Structures, WUT, which is changed to Wuhan University of Sciences and Technology. The main research interests and technical expertise are in wind engineering, earthquake engineering, structural dynamics, vibrations and stability of structures, structural reliability, structural control, expert system for design of buildings and structures. His research in these fields has resulted over 500 journal papers and published 14 books. He got two national awards, two awards of the first class of the scientific and technological progress from the Ministry of Education of China, the first-class award of scientific and technological progress of Hubei province, and several second awards.

Slow Variation and Sudden Variation

It is well known that structural stiffness and load will be changed in the life of engineering structures. In general, the variation of structural stiffness is very slow. This type of variation is called “slow variation”. The variation of static load in the life of engineering structure is also belong to “slow variation”. But the variation of earthquake force and gust wind force are very fast. This type of variation is called “sudden variation”. The time dependent dynamic reliability of engineering structures for the cases of “slow variation” and “sudden variation” have been proposed.

Static Reliability

According China Code the structural reliability index is given by:

$$\beta = \frac{\mu_2}{\sigma_2} \tag{1}$$

where,

μ_2 – the mathematic expect of structural resistance

σ_2 – standard deviation of structural resistance

considering the structural resistance is changed in its life, the structural reliability index must be expressed as:

$$\beta(n) = \frac{\mu_2(n)}{\sigma_2(n)} \tag{2}$$

where,
$n -$ the nth year

i.e., $\mu_2(n)$ and $\sigma_2(n)$ represent the nth year mathematic expect and the standard deviation of structural resistance, respectively.
$\beta(n) -$ the nth year structural reliability index

Crossing of a Random Process with a Non-Random Time-Dependent Demarcation Line

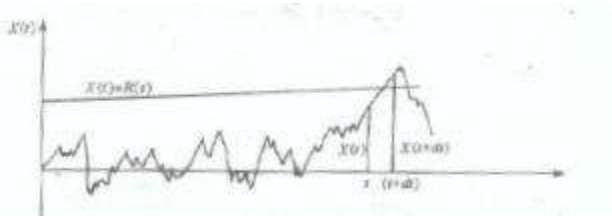

Fig. 1 Crossing of random process $X(t)$ with time-dependent demarcation line.

To assume $X(t)$ is a random process with a zero average shown in Fig 1, $R(t)$ represents a lineally strengthening resistance of a structure, i.e., the resistance is increased with time, $\dot{R}(t) > 0$.

Considering the crossing times of $X(t)$ with $R(t)$ at the internal $[t, t + dt]$ with positive slope (Fig 1), it is obvious that:

$$\gamma_R^+ dt = P\left[X(t) < R(t) \bigcap X(t + dt) > R(t + dt)\right] \tag{3}$$

where, γ_R^t is the crossing times per second of $X(t)$ with positive slope.

As well known as that $X(t + dt)$ and $R(t + dt)$ can be expressed as:

$$X(t + dt) \approx X(t) + X(t)dt$$
$$R(t + dt) \approx R(t) + R(t)dt$$

Substituting above two equations into Eq. (3), we have:

$$\gamma_R^+ dt = P\{R(t) \bigcap [X(t) + X(t)dt) > R(t) + R(t)dt)]\} \tag{4}$$

Since, $X(t) - R(t) > \frac{R(t) - X(t)}{dt}$,

$$\gamma_R^+(t) = \int_R^\infty (\dot{X} - \dot{R})\, f_{x\dot{x}}(R, \dot{X}, t)dx \tag{5}$$

Using the same way gives the crossing times per second of X(t) with negative slope:

$$\gamma_R^-(t) = \int_{-\infty}^R |\dot{X} - \dot{R}|\, f_{x\dot{x}}(R, \dot{X}, t)d\dot{x} \tag{6}$$

Obviously, the crossing times per second of X(t) with the positive and negative slope, γ_R, can be obtained from above two equations as follows:

$$\gamma_R(t) = \int_{-\infty}^\infty \left|\dot{X} - \dot{R}\right| f_{xx}(R, x, t)dx \tag{7}$$

If X(t) is a stationary Gauss process with zero average, then

$$\gamma_R^+(t) = \gamma_R^-(t) = \frac{A}{2\pi}\frac{\sigma_{\dot{x}}}{\sigma_x}\exp\left(-\frac{R^2(t)}{2{\sigma_x}^2}\right) \tag{8}$$

$$\gamma_R(t) = \frac{A}{\pi}\frac{\sigma_{\dot{x}}}{\sigma'_x}\exp\left(-\frac{R^2(t)}{2{\sigma_x}^2}\right) \tag{9}$$

In which,

$$A = \exp\left(-\frac{\dot{R}^2}{2{\sigma_x}^2}\right) - \sqrt{2\pi}\frac{\dot{R}}{\sigma_x}\Phi\left(-\frac{\dot{R}}{\sigma_x}\right) \tag{10}$$

$A =$ constant when $\dot{R}$ = constant.
$\Phi\left(-\frac{\dot{R}}{\sigma_x}\right)$ is a distribution function of normalization Gauss process.

It can be seen from Eq. (10) that:

$A = 1$, if $\dot{R} = 0$
i.e., if the structural resistance is not variation in the whole loading process,
$A > 1$, if $\dot{R} < 0$
i.e., if the structural resistance is lineally decreased with time in the whole loading process,
$A < 1$, if $\dot{R} > 0$
i.e., if the structural resistance is lineally increased with time in the whole loading process.

Time-dependent dynamic reliability based on first passage failure criteria under Poisson hypothesis is:

$$P_{s1}(n, T) = \exp[-\frac{A\sigma_{\dot{x}}}{2\pi\sigma_x}\left[\exp\left(-\frac{R^2}{2{\sigma_x}^2}\right)\right] \tag{11}$$

For single boundary line, where T is the duration of X(t).

$$P_{s2}(n,T) = \exp\{-\frac{A\sigma_{\dot{x}}}{2\pi\sigma_x}\left[\exp\left(-\frac{{R_{n1}}^2}{2{\sigma_x}^2}\right) + \exp\left(-\frac{{R_{n2}}^2}{2{\sigma_x}^2}\right)\right]\} \quad (12)$$

For double-boundary lines, when $R_{n1} = R_{n2} = R_n$, then

$$P_{n2}(n) = \exp[-\frac{A\sigma_{\dot{x}}}{2\pi\sigma_x} exp\left(-\frac{{R_n}^2}{2{\sigma_x}^2}\right)] \quad (13)$$

If the crossing process of X(x) with R(t) is Markov process, then

$$P_{s1}(n,T) = \exp\left[-\frac{A\sigma_{\dot{x}}T}{2\pi\sigma_x}\exp\left(-\frac{{R_{n1}}^2}{2{\sigma_x}^2}\right)\frac{1-\exp\left(-\sqrt{\frac{\pi}{2}}q\frac{R_{n1}}{\sigma_x}\right)}{1-\exp\left(-\frac{{R_{n1}}^2}{2{\sigma_x}^2}\right)}\right]$$

$$P_{s2}(n,T) = \exp\{-\frac{A\sigma_{\dot{x}}T}{2\pi\sigma_x}[\exp\left(-\frac{{R_{n1}}^2}{2{\sigma_x}^2}\right)\frac{1-\exp\left(-\sqrt{\frac{\pi}{2}}q\frac{R_{n1}}{\sigma_x}\right)}{1-\exp\left(-\frac{{R_{n1}}^2}{2{\sigma_x}^2}\right)}$$

$$+\exp\left(-\frac{{R_{n2}}^2}{2{\sigma_x}^2}\right)\frac{1-\exp\left(-\sqrt{\frac{\pi}{2}}q\frac{R_{n2}}{\sigma_x}\right)}{1-\exp\left(-\frac{{R_{n2}}^2}{2{\sigma_x}^2}\right)} \quad (14)$$

When $R_{n1} = R_{n2} = R_n$, then

$$P_{s2}(n,T) = \exp\left[-\frac{A\sigma_{\dot{x}}T}{\pi\sigma_x}\exp\left(-\frac{{R_n}^2}{2{\sigma_x}^2}\right)\frac{1-\exp\left(-\sqrt{\frac{\pi}{2}}q\frac{R_n}{\sigma_x}\right)}{1-\exp\left(-\frac{{R_n}^2}{{\sigma_x}^2}\right)}\right] \quad (15)$$

where,

$$q = \sqrt{1-\frac{{\alpha_1}^2}{\alpha_0\alpha_2}},\ \alpha_i = E\left[X^i\right], \quad i = 0,1,2, \text{ if,}$$
$$R_n(t) = \alpha(n,t)R_0 \quad (16)$$

where,

$\alpha(n,t)$ – a determinate function
R_0 – a random variable that is initial resistance of a structure
then,

$$for\ single\ boundary\ line: P_{s1}(n,T)$$
$$= \exp\{-\frac{A\sigma_{\dot{x}}T}{2\pi\sqrt{{\sigma_x}^2+{\sigma_{R_{n1}}}^2}}\exp\left[-\frac{{\bar{R}_{n1}}^2}{2\left({\sigma_x}^2+{\sigma_{R_{n1}}}^2\right)}\right]\} \quad (17)$$

$$P_{s2}(n,T) = \exp\{-\frac{A_1\sigma_{\dot{x}}T}{2\pi\sqrt{{\sigma_x}^2+{\sigma_{R_{n1}}}^2}}\exp\left[-\frac{{\bar{R}_{n1}}^2}{2({\sigma_x}^2+{\sigma_{R_{n1}}}^2)}\right] - \frac{A_2\sigma_{\dot{x}}T}{2\pi\sqrt{{\sigma_x}^2+{\sigma_{R_{n2}}}^2}}\exp\left[-\frac{{\bar{R}_{n2}}^2}{2({\sigma_x}^2+{\sigma_{R_{n2}}}^2)}\right]\} \quad (18)$$

$$for\ double\ boundary\ lines: P_{s_n}(n,T) = \exp\{-\frac{A\sigma_{\dot{x}}T}{\pi\sqrt{{\sigma_x}^2+{\sigma_{R_n}}^2}}\exp\left[-\frac{{\bar{R}_n}^2}{2({\sigma_x}^2+{\sigma_{R_n}}^2)}\right]\} \quad (19)$$

for the case that $R_{n1} = R_{n2} = R_n$.

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Using Transparent Material for Simulating Bubbles Formation in the Mushy Zone

by Qingyou Han, Member EUAS

Short Biography

Dr. Qingyou Han is a Professor of Mechanical Engineering Technology, the Foundry Education Foundation (FEF) Key Professor at Purdue University, and Director of the Purdue Center for Materials Processing Research at Purdue University. He received his B.S. degree from Wuhan Institute of Technology, his M.S. degree from University of Science and Technology Beijing, and his Ph.D. degree from The University of Oxford. Before joining Purdue University, Dr. Han was the P.I. of the Aluminum and Casting Programs and a research engineer at Oak Ridge National Laboratory. His research interests include solidification and casting processing of metals and alloys, composite processing, and the application of high-intensity ultrasonic vibration for material processing. His research program has received funding from industry, National Science Foundation, and the U.S. Department of Energy. He has over 200 scientific publications, 8 patents, and numerous presentations to his credit, and has organized or co-organized several international symposia in his areas of research.

Using Transparent Material for Simulating Bubbles Formation in the Mushy Zone

Qingyou Han

The John Hunt International Symposium, 2011

Abstract

Bubbles usually form during solidification of alloys having a large solubility of gas in the liquid but a negligible solubility of gas in the solid. These bubbles become pores in a solidified casting, deteriorating the mechanical properties, notably the fatigue life of the alloys. *In situ* observation of pore formation in metallic alloys is difficult because of their opacity. Transparent organic materials, which were first used by Hunt and his co-workers for the physical simulation of metal solidification, are ideal for the study of bubble formation in the mushy zone. This article describes the behaviour of bubbles in the mushy zone of cyclohexane under directional solidification conditions. It can be observed that worm-like bubbles are formed at low growth rates of the solid. At high growth rates, radical motion of bubbles in the mushy zone occurs. Often, bubbles jump at great speeds from location to location towards higher temperature regions in the mushy zone. If the growth rate of the solid is suddenly decreased, eruption of bubbles often occurs at the freezing front. It is believed that these types of radical motion of bubbles in the mushy zone strongly affect the final distribution and the size of pores in a solidifying casting.

Ultrasonic Processing of Materials

Qingyou Han

Abstract

Irradiation of high energy ultrasonic vibration in metals and alloys generates oscillating strain and stress fields in solids, and introduces nonlinear effects such as cavitation, acoustic streaming, and radiation pressure in molten materials. These nonlinear effects can be utilized to assist he conventional materials processing processes. This article describes recent research at Purdue University using high intensity ultrasonic vibrations for deagssing molten aluminum, processing particulate reinforced metal matrix composites, refining metals and alloys during solidification process, and producing bulk nanostructures in solid metals and alloys.

Particle Pushing during Solidification of Metals and Alloys

Qingyou Han, Meng Wang and Fei He

Abstract

The most inexpensive process for making metal matrix composite (MMC) components is the casting process. This process involves the mixing of reinforcement particles in molten metal using a stirrer. The molten metal containing a fraction of ceramic particles is then cast into net shaped component. During the solidification of MMC, particles are either rejected or engulfed by the growing solid phase. Theories have been proposed on the mechanisms of particle pushing by a freezing front. This work evaluates these mechanisms. Specially selected alloy systems, an Al-Ti-B master alloy, and pure aluminum metal containing nano-particles, were used to evaluate particle pushing under various solidification conditions. The final distribution of the particles in ingots is examined. It is concluded that most of the particles are pushed by the dendritic solid liquid interface under cooling conditions varying a few orders of magnitude. Mechanical disturbance, such as vibration or fluid flow in the remaining liquid of the mushy zone, promotes particle pushing by the growing solid.

The Mechanism of Die Solderning in Aluminum Die Casting

Qingyou Han

Abstract

Soldering is a unique casting defect associated with die casting or metal mold casting of aluminum alloys. It occurs when molten aluminum sticks or solders the surface of the die steel and remains there after the ejection of the casting, causing surface defect and dimensional inaccuracy of the castings and increased machine downtime. Soldering occurs easily when a bare die steel mold is used for die casting of aluminum alloys. When molten aluminum comes in contact with the die steel at a temperature higher than a critical temperature, the iron and aluminum atoms diffuse into each other, forming a series of

intermetallic phases and a liquid aluminum-rich fcc phase. This liquid phase exists between intermetallic phases. On cooling the liquid fcc phase solidifies on the intermetallic phases and grows into the casting, resulting in soldering. The critical temperature is the eutectic temperature near the aluminum corner of the phase diagram. If the die is protected using a nonreactive ceramic coating, soldering starts at locations where local coating failure occurs. Molten aluminum comes into contact with die steel through the coating failure locations and eats into the steel matrix, forming small pits. As these small pits grow, the coating is gradually removed and soldering becomes more severe. Details of step for die soldering on a bare steel die and on a coated die material are discussed.

Surface Nanocrystallization and Numerical Modelling of AISI-1018 Steel by Means of Ultrasonic Shot Peening

Fei Yin, Qingyou Han, Xiaoming Wang, Sergey Suslov, Lin Hua

Abstract

Surface nanocrystallization of AISI-1018 steel was successfully realized by ultrasonic shot peening technique. A nanocrystalline surface layer was fabricated on the peened surface of AISI-1018 plate. The deformation layer and nano-sized grains were observed and characterized by means of Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM). Experimental evidence indicates that after ultrasonic shot peening treatment, the initial coarse-grained structural at the top surface layer was refined into equiaxed ultrafine grains with random crystallographic orientation and the elongated grains were observed at the sub-surface layer as well. In addition, an analytical algorithm was proposed to simulate the surface topography and strain distribution of the sample after multiple-impacts during ultrasonic shot peening process. The proposed algorithm was verified by the physical experiments and the simulation results show a reasonable agreement with the experimental results.

Contributions in Nutritional Epidemiology and Clinical Nutrition Research

by Michele Forman, Member EUAS

Short Biography
Michele R. Forman, Ph.D, FACE
Distinguished Professor and Department Head
Department of Nutrition Science
College of Health and Human Science
Purdue Center for Cancer Research
Purdue University
In 2017, Dr. Michele Forman joined Purdue University, as the Head Department of Nutrition Science. She is currently a member of the Purdue Cancer Center, the Center for Aging and Life Course and the Public Health Program. In 2018, she received a Distinguished Professorship at Purdue University, a Special Award for Epidemiologic Research on Critical and Sensitive Windows for Health across the Lifespan, American College of Epidemiology, and the H.A. Tyroler Distinguished Alumni Award in Epidemiology, University of North Carolina Gillings School of Public Health, Chapel Hill, N.C.. She is a University Scholar of the American University of Beirut, Lebanon.

Dr. Forman's career focuses on nutritional epidemiology and clinical nutrition research across the globe with an emphasis on early life exposures and risk for chronic disease as well as the role of nutrition in growth and health across the life course. As her research foci have shifted from low birth-weight to chronic disease, the still point of the compass has remained fixed; she examines the developmental origins of disease. Much of her research is designed either as a longitudinal prospective cohort study that spans the peri-conceptional period through adulthood or dietary interventions in the free-living state or under controlled feeding conditions or randomized clinical trials. Her laboratory addresses nutritional assessment of individuals from infancy through adulthood; and tests dietary interventions amongst high risk groups such as chronic renal disease patients.

She has over 180 peer-reviewed publications, numerous invited presentations nationally and internationally, is on many institutional committees, advisory boards (e.g. Board of Directors American College of Epidemiology, Board of the Gillings School of Public Health at the University of North Carolina, her alma mater, and chaired program committees for ASPO). She has mentored over 80 postdoctoral fellows, graduate and undergraduate students who have posts at the NIH-NCI, NICHD, FDA, Kaiser Permanente, Emory University Rollins School of Public Health and other prestigious institutions.

Her current research has three genre: life course epidemiology; dietary interventions in adults to prevent chronic disease; and the role of the epigenome in health. Her life course research examines the role of early life exposures on health

across the life course demonstrating for example the strong signal from gestation weight gain on risk for obesity across the life course and early menarche; and how physical activity in pregnancy delays age at menarche. She has studied preeclampsia in pregnancy and its effects on the mother and index offspring over the life course. Specifically, she is the PI for a study of the effects of preeclampsia on pubertal and nutritional development in Stavanger, Norway that is directed at the question why preeclampsia is associated with lower risk for breast cancer in the mother and daughter and lower risk for prostate and testicular cancers in the sons of the index pregnancy. We have reported that daughters of the PE pregnancy delay breast development but have advanced pubarche compared to daughters of normotensive pregnancies; that PE mothers who breast feed have lower insulin and glucose levels but higher risk for hypertension and cardiovascular disease 11 years postpartum as do their offspring, that PE offspring have higher SBP than peers.

Her research in dietary fruit-vegetable interventions and biomarkers of disease is designed as controlled feeding studies or interventions in the free-living state. Under controlled feeding conditions, her team has examined the cyclic fluctuation of hormones with carotenoids and lipids with and without alcohol intake. Results indicate major changes in the carotenoid distribution on lipoprotein carriers by phase of the menstrual cycle and the alcohol alters the carotenoid profiles over the cycle. In the free-living state her team conducted field trials to assess whether a low fat, high fruit and vegetable diet delays time till dialysis or reduced kidney function in patients with chronic renal disease as well as co-I on the Polyp Prevention Trial, a dietary randomized trial of colon polyp patients to reduce recurrence. Kidney patients are apt to change their diet under mindful feeding conditions and thereby lower their weight and enhance their serum profile of antioxidants.

Diet and Epigenetic Influences on Health. As part of an ongoing collaboration, we have investigated the epigenetic alterations from diet in pregnancy and infancy on the health of the index offspring. This research has led to understanding how prenatal and folate supplements influence obesity, how breast feeding can modify epigenetic alterations and explore the role of nutrition through the lens of the epigenome in humans.

Dr. Forman has a laboratory of three doctoral students, ten undergraduate students and conducts field studies abroad and in the U.S. Please visit her profile at the Purdue University College of Health and Human Sciences to learn more about her work and that of her department.

Maximizing Life Saving through Better Placement of Defibrillators

by Zuo-Jun Max Shen, Member EUAS

Short Biography

Zuo-Jun Max Shen got his PhD from the Department of Industrial Engineering and Management Sciences at Northwestern University. He received the CAREER award from National Science Foundation (US), the Franz Edelman Finalist Award from the Institute of Operations Research and Management Sciences (INFORMS), won several best paper awards, and was elected Fellow of INFORMS in 2018. He is a professor and Department Chair in the Department of Industrial Engineering and Operations Research, and a professor in the Department of Civil and Environmental Engineering, at the University of California, Berkeley. He is also an honorary professor at Tsinghua University and the Co-Director of the Environment and New Energy Center at Tsinghua-Berkeley Institute. He has been active in the following research areas: integrated supply chain design and management, logistics automation and optimization, Energy Systems Optimization, and Transportation System Planning and Optimization, and has overseeing many projects funded by the National Science Foundation, California Department of Transportation and other entities, including the CAREER award from National Science Foundation in 2003. He is currently the senior/area/associate editor for several leading journals in the areas of management science and optimization, such as Management Science, Operations Research, Manufacturing & Service Operations Management, Production and Operations Management, Naval Research Logistics, IIE Transactions, Decision Sciences, and Asia-Pacific Journal of Operational Research. His paper, "A Joint Location-Inventory Model", published in Transportation Science in 2003, was voted one of Transportation Science's most impactful papers in the 50-year history of the journal. His book, Fundamentals of Supply Chain Theory, co-authored with Larry Snyder, won the 2012 IIE/Joint Publishers Book-of-the-Year Award.

Maximizing Life Saving through Better Placement of Defibrillators

Sudden cardiac arrest, which occurs when the heart unexpectedly stops beating, kills more than 400,000 people in the U.S. and Canada every year. Death happens within minutes if not treated, and 92 percent who suffer an attack outside of a hospital don't survive.

The use of automated external defibrillators, or AEDs, which deliver a strong electric shock to jolt the heart back into action, can dramatically improve survival rates. But the key is quick action; the American Heart Association says that when defibrillation is applied within five minutes, the survival rate can be as high as 45 percent. The units can

cost about $3,000 each. An industry estimate puts the number of AEDs in the U.S. at 2.4 million.

Because AEDs can be used by untrained bystanders, health officials want to see them widely deployed in workplaces, malls, restaurants, subway stations and other public places. Research has found that access to AEDs drastically reduces the delay in treating cardiac patients. One estimate suggests that widespread deployment of defibrillators could save as many as an additional 4,000 lives per year in the U.S.

The trouble is, AEDs are rarely used. There are lots of reasons, but one is that the devices aren't always located where they can be reached quickly in an emergency.

That's the problem tackled by University of Toronto's Timothy C.Y. Chan, UC Berkeley's Zuo-Jun (Max) Shen and UCLA Anderson's Auyon Siddiq in a paper published in *Operations Research*. The authors propose a model for deploying publicly accessible AEDs where they're most likely to be used by taking into account where cardiac arrests *might* occur, not just where they happened in the past. With the model, the authors say, health officials can position the devices in a way that "can improve survival rates by shortening the distance to the nearest AED."

Typically, AEDs are placed where people congregate, such as shopping malls or office buildings, but these aren't always easily accessible when an attack occurs out on the street. Researchers have tried to improve the availability of AEDs by looking at the site of previous attacks. But given the random nature of cardiac arrests, this method fails to consider where they could take place in the future. Another approach is to estimate the number of incidents that occur within a certain distance of an AED location. This can make the devices accessible to the average patient, but can leave many victims dangerously distant from the nearest device.

With their model, Chan, Shen and Siddiq seek to improve on existing methods by addressing the uncertainty about where cardiac arrests might occur in the future and by making sure the most distant victims are still near an AED.

Normally, modeling all the possible locations would be a computational nightmare. The authors devised an efficient way to solve the problem by considering only a subset of the millions of alternatives. This, the research suggests, is enough to come up with a model that performs better than one that bases siting decisions on the location of past cardiac

arrests.

The authors considered the problem of deploying 30 AEDs in Toronto's densely populated financial district. They mapped the 43 cardiac arrest events that occurred in public areas from January 2006 to April 2013, and then identified 120 public places, such as restaurants or shops, where AEDs could be deployed. They divided the area into 15 equally shaped cells and, using their model, projected where cardiac arrests could occur. By comparing distances, they then determined the optimal placement of AEDs.

When compared with a model that used historical cardiac arrests, the authors' model reduced the distance between an attack and the nearest AED by at least 9 percent on average and as much as 20 percent. Using Google Maps to measure walking distances, they estimated that with their model, cardiac arrests on average would occur 12 meters closer to the nearest AEDs than would those based on past attacks. For patients that were the most distant, the authors' model placed devices 11 meters closer.

While the approach is largely theoretical, it shows that it's possible to come up with a way to deploy AEDs that's better than existing methods, the authors suggest. It could be especially effective when combined with a "crowdsourcing" approach to responding to cardiac emergencies. Mobile apps, such as an application developed by San Francisco-based PulsePoint Foundation, can be used when a cardiac arrest occurs to alert nearby volunteers and identify the nearest AED, potentially shaving crucial minutes off response times.

"In a setting where lay responders are recruited to intervene during a cardiac arrest," the authors write, "it is even more critical that AEDs are tactically located throughout an urban area."

Reference

Chan, T.C.Y., Shen, Z., & Siddiq, A. (2017). Robust defibrillator deployment under cardiac arrest location uncertainty via row-and-column generation. *Operations Research, 66*(2), 358–379. doi: 10.1287/opre.2017.1660

Innovative Research on Cancer's Oncology

by Dean W. Felsher, Member EUAS

Short Biography

***Academic History**:*
Colleges and University
9/81-7/85 University of Chicago, B.A.
7/85-7/92 University of California, Los Angeles, M.D., PhD.
7/92-6/94 Hospital of the University of Pennsylvania, Resident, Internal Medicine
7/94-6/99 University of California, San Francisco, Fellow, Hematology-Oncology
Scholarships and Honors
1985 Special Honors, Chemistry, University of Chicago
1992 Emil Bogen Research Award for Excellence in Science
1985-1992 Medical Scientist Training Program
Residency and Post-Doctoral Training
7/92-6/94 Resident, Hospital of the University of Pennsylvania, Internal Medicine
7/94-6/99 Fellow, University of California, San Francisco, Hematology-Oncology
7/95-6/99 Fellow, University of California, San Francisco, J. Michael Bishop's Laboratory
Board Certification
1996 Internal Medicine
1998 Medical Oncology
Employment History:
12/97-7/98 Clinical Instructor, Department of Medicine, UCSF
7/98-9/99 Assistant Adjunct Professor, Step I, Department of Medicine, UCSF
9/1/99-12/1/99 Acting Assistant Professor, Division of Oncology, Department of Medicine, Stanford University
12/1/99- Assistant Professor, Division of Oncology, Department of Medicine, Stanford University
11/1/01- Assistant Professor, Division of Oncology, Departments of Medicine and Pathology, Stanford University
2/1/07- Associate Professor, Division of Oncology, Departments of Medicine and Pathology, Stanford University
8/01/12- Professor, Division of Oncology, Departments of Medicine and Pathology, Stanford University.
Public and Professional Service:
Departmental Affiliations
Division of Oncology, Department of Medicine, Stanford University
Department of Pathology, Stanford University
Center for Clinical Immunological Sciences, Stanford University
Medical Scientist Training Program, Stanford University
Digestive Disease Center, Member, Stanford University
Stanford Comprehensive Cancer Center
Molecular Imaging Program
Tumor Biology Training Program
Graduate Programs
2000- Cancer Biology, Stanford University
2001- Immunology, Stanford University
Research and Professional Experience
7/85-7/92 Medical Scientist Training Program, UCLA
7/87-7/91 Graduate Student, MBI, UCLA, advisor: Dr. Jonathan Braun
7/92-6/94 Resident, Hospital of the University of Pennsylvania
7/94-6/97 Fellow, Division of Hematology-Oncology, UCSF
7/95-6/99 Fellow, Hooper Foundation, advisor: Dr. J. Michael Bishop
7/98-9/99 Assistant Adjunct Professor, Department of Medicine, UCSF
9/99- Assistant Professor, Department of Medicine, Stanford University

11/01- Assistant Professor, Departments of Medicine and Pathology, Stanford University
2/1/07- Associate Professor, Division of Oncology, Departments of Medicine and Pathology, Molecular Imaging, Stanford University
09/01/12- Professor, Division of Oncology, Departments of Medicine and Pathology, Molecular Imaging, Stanford Imaging
10/01/16- Director of Research, Division of Oncology, Stanford University
Editorial Board
2008- Cancer Biology and Therapy
2009- Journal of Clinical Investigation
2009- Chinese Journal of Cancer
2010- Cancer Research
2010- Hematology Oncology
2010- OncoTarget
2010 Cancer Research, Associate Editor of Breaking Advances
2010 International Journal of Oncology
2012 OncoImmunology – Journal of the European Academy of Tumor Immunology
2012 Oncogene, Nature Publishing Group, Senior Editor
2013 Cancer Immunology Research – AACR Journal
2013 Cancer Hallmarks
2018 AACR, Senior Editor for Cancer Research

MYC Activation Is a Hallmark of Cancer Initiation and Maintenance

Meital Gabay, Yulin Li, and Dean W. Felsher

Cold Spring Harb Perspect Med 2014;4:a014241

The MYC proto-oncogene has been implicated in the pathogenesis of most types of human tumors. MYC activation alone in many normal cells is restrained from causing tumorigenesis through multiple genetic and epigenetically controlled checkpoint mechanisms, including proliferative arrest, apoptosis, and cellular senescence. When pathologically activated in a permissive epigenetic and/or genetic context, MYC bypasses these mechanisms, enforcing many of the "hallmark" features of cancer, including relentless tumor growth associated with DNA replication and transcription, cellular proliferation and growth, protein synthesis, and altered cellular metabolism. MYC mandates tumor cell fate, by inducing stemness and blocking cellular senescence and differentiation. Additionally, MYC orchestrates changes in the tumor microenvironment, including the activation of angiogenesis and suppression of the host immune response. Provocatively, brief or even partial suppression of MYC back to its physiological levels of activation can result in the restoration of intrinsic checkpoint mechanisms, resulting in acute and sustained tumor regression, associated with tumor cells undergoing proliferative arrest, differentiation, senescence, and apoptosis, as well as remodeling of the tumor microenvironment, recruitment of an immune response, and shutdown of angiogenesis. Hence, tumors appear to be "addicted" to MYC because of both tumor cell–intrinsic, cell-autonomous and host-dependent, immune cell–dependent mechanisms.
Both the trajectory and persistence of many human cancers require sustained MYC activation. Multiscale mathematical modeling may be useful to predict when tumors will be addicted to MYC. MYC is a hallmark molecular feature of both the initiation and maintenance of tumorigenesis.

MYC regulates the antitumor immune response through CD47 and PD-L1

Stephanie C. Casey, Ling Tong, Yulin Li, Rachel Do, Susanne Walz, Kelly N. Fitzgerald, Arvin M. Gouw, Virginie Baylot, Ines Gütgemann, Martin Eilers, Dean W. Felsher

Cancer Biology, VOL 352 ISSUE 6282, 227-231, 2016.

The MYC oncogene codes for a transcription factor that is overexpressed in many human cancers. Here we show that MYC regulates the expression of two immune checkpoint proteins on the tumor cell surface: the innate immune regulator CD47 (cluster of differentiation 47) and the adaptive immune checkpoint PD-L1 (programmed death–ligand 1). Suppression of MYC in mouse tumors and human tumor cells caused a reduction in the levels of CD47 and PD-L1 messenger RNA and protein. MYC was found to bind directly to the promoters of the Cd47 and Pd-l1 genes. MYC inactivation in mouse tumors down-regulated CD47 and PD-L1 expression and enhanced the antitumor immune response. In contrast, when MYC was inactivated in tumors with enforced expression of CD47 or PD-L1, the immune response was suppressed, and tumors continued to grow. Thus, MYC appears to initiate and maintain tumorigenesis, in part, through the modulation of immune regulatory molecules.

Alteration of the lipid profile in lymphomas induced by MYC overexpression

Livia S. Eberlina, Meital Gabayb, Alice C. Fanb, Arvin M. Gouwb, Robert J. Tibshirani, Dean W. Felsher and Richard N. Zare

PNAS vol. 111, no. 29, 10450–10455 , 2014

Overexpression of the v-myc avian myelocytomatosis viral oncogene homolog (MYC) oncogene is one of the most commonly implicated causes of human tumorigenesis. MYC is known to regulate many aspects of cellular biology including glucose and glutamine metabolism. Little is known about the relationship between MYC and the appearance and disappearance of specific lipid species. We use desorption electrospray ionization mass spectrometry imaging (DESI-MSI), statistical analysis, and conditional transgenic animal models and cell samples to investigate changes in lipid profiles in MYC-induced lymphoma. We have detected a lipid signature distinct from that observed in normal tissue and in rat sarcoma-induced lymphoma cells. We found 104 distinct molecular ions that have an altered abundance in MYC lymphoma compared with normal control tissue by statistical analysis with a false discovery rate of less than 5%. Of these, 86 molecular ions were specifically identified as complex phospholipids. To evaluate whether the lipid signature could also be observed in human tissue, we examined 15 human lymphoma samples with varying expression levels of MYC oncoprotein. Distinct lipid profiles in lymphomas with high and low MYC expression were observed, including many of the lipid species identified as significant for MYC-induced animal lymphoma tissue. Our results suggest a relationship between the appearance of specific lipid species and the overexpression of MYC in lymphomas.

MYC oncogene overexpression drives renal cell carcinoma in a mouse model through glutamine metabolism

Emelyn H. Shroffa, Livia S. Eberlinb, Vanessa M. Dangc, Arvin M. Gouwa, Meital Gabaya, Stacey J. Adama, David I. Bellovina, Phuoc T. Trand, William M. Philbrick, Adolfo Garcia-Ocanag, Stephanie C. Caseya, Yulin Lia, Chi V. Dangc, Richard N. Zareb,1, and Dean W. Felshera

PNAS vol. 112 , no. 21, 6539–6544, 2015

The MYC oncogene is frequently mutated and overexpressed in human renal cell carcinoma (RCC). However, there have been no studies on the causative role of MYC or any other oncogene in the initiation or maintenance of kidney tumorigenesis. Here, we show through a conditional transgenic mouse model that the MYC oncogene, but not the RAS oncogene, initiates and maintains RCC. Desorption electrospray ionization–mass-spectrometric imaging was used to obtain chemical maps of metabolites and lipids in the mouse RCC samples. Gene expression analysis revealed that the mouse tumors mimicked human RCC. The data suggested that MYC-induced RCC up-regulated the glutaminolytic pathway instead of the glycolytic pathway. The pharmacologic inhibition of glutamine metabolism with bis-2-(5-phenylacetamido-1,2,4-thiadiazol-2-yl) ethyl sulfide impeded MYC-mediated RCC tumor progression. Our studies demonstrate that MYC overexpression causes RCC and points to the inhibition of glutamine metabolism as a potential therapeutic approach for the treatment of this disease.

Oncogene KRAS activates fatty acid synthase, resulting in specific ERK and lipid signatures associated with lung adenocarcinoma

Arvin M. Gouwa, Livia S. Eberlinc, Katherine Margulisc, Delaney K. Sullivana, Georgia G. Toala, Ling Tonga, Richard N. Zarec and Dean W. Felshera

PNAS vol. 114, no. 17, 4300–4305, 2017

KRAS gene mutation causes lung adenocarcinoma. KRAS activation has been associated with altered glucose and glutamine metabolism. Here, we show that KRAS activates lipogenesis, and this activation results in distinct proteomic and lipid signatures. By gene expression analysis, KRAS is shown to be associated with a lipogenesis gene signature and specific induction of fatty acid synthase (FASN). Through desorption electrospray ionization MS imaging (DESI-MSI), specific changes in lipogenesis and specific lipids are identified. By the nanoimmunoassay (NIA), KRAS is found to activate the protein ERK2, whereas ERK1 activation is found in non–KRAS-associated human lung tumors. The inhibition of FASN by cerulenin, a small molecule antibiotic, blocked cellular proliferation of KRAS-associated lung cancer cells. Hence, KRAS is associated with activation of ERK2, induction of FASN, and promotion of lipogenesis. FASN may be a unique target for KRASassociated lung adenocarcinoma remediation.

Pricing Options with VG Model using FFT

by Andrey Itkin, Member EUAS

Short Biography

I am currently working as a Director, Senior Quantitative Research Associate at Bank of America, Merrill Lynch and Adjunct Professor of computational and algorithmic finance at Department of Risk and Financial Engineering, Tandon School of Engineering of NYU.
My academic working experience includes positions of leading researcher with the Institute of Theoretical Astronomy of the Russian Academy of Sciences, senior researcher at St.Petersburg Technical University, Visiting Fellow at Department of Chemistry and Biochemistry at UCLA, and at Moscow Aviation University where for 14 years I worked as a Full Professor at the Department of Applied Mathematics and Physics. I also occupied senior managerial positions at the Institute of High Performance computing and Databases of the Russian Ministry of Science (as the Director of Operation and Research of the Moscow Branch) and at the International Institute for Problems of the Asteroid Hazard (as the Deputy Director). I also served as an expert of Russian-American committees on scientific collaboration, supercomputing and digital libraries.
I received PhD in physics of liquids, gases and plasma, and degree of Doctor of Science in computational molecular physics. During my academic carrier I published 2 monographs and 10 preprints on chemical and theoretical physics and math finance, and more than 100 papers including articles in peer-reviewed journals and proceedings of international conferences on chemical, molecular and computational physics, math finance and programming. My recent book "Pricing Derivatives under Levy Models. Modern Finite-Difference and Pseudo-Differential Operators Approach" was published by Springer in 2017.
I am an Associate Editor at the International Journal of Computer mathematics and the Journal of Derivatives. Also I was a guest editor of

1. *Special issue - Computational Methods in Finance (the International Journal of Computer Mathematics, vol.92, issue 12, 2015).*
2. *Special issue - Computational and algorithmic finance (Computational Science, vol.24, 2018).*
3. *Special issue - Physics of Financial Derivatives (the Journal of Derivatives) - current work*

and also help as a reviewer of multiple journals. I was an organizier of two international workshops on computational and algorithmic finance as a part of ICCS.
After moving to finance I occupied multiple positions in this industry: Head of Quantitative Development at Numerix, senior consultant at JPMorgan, Director of Financial Engineering at HAP Capital and Chicago Trading Company, Head of Quantitative Strategies and partner at Volant Trading LLC, Senior Quantitative Engineer at Amaranth Group, Project Manager at Bloomberg L.P. (R&D quantitative group) and Programming Manager at Thomson Financial.
I am also a member of multiple professional associations in finance and physics
EDUCATION AND DEGREES

- *Dr. of Science in computational/molecular physics, St.Petersburg University*
- *BS in Economics, Moscow Politic University*
- *Ph.D. in mechanics of gases, fluids and plasma, Moscow Aviation Technical University*
- *MS in Applied mathematics and physics, Moscow Aviation Technical University*
- *Physics and Mathematics school of Moscow Institute of Physcis and Technology*

Pricing Options with VG Model using FFT

A. Itkin

Extended version prepared for the VG Conference

We discuss various analytic and numerical methods that have been used to get option prices within a framework of the VG model. We show that some popular methods, for instance, Carr-Madan's FFT method could blow up for certain values of the model parameters even for European vanilla option. Alternative methods - one originally proposed by Lewis, and Black-Scholes-wise method are considered that seem to work fine for any value of the VG parameters. Test examples are given to demonstrate efficiency of these methods. Convergence of all methods is also discussed.

Pricing swaps and options on quadratic variation under stochastic time-change models discrete observations case

A. Itkin, P. Carr

Review of Derivatives Research, 2010, Vol.13, N.2,, p.141-176.

We use a forward characteristic function approach to price variance and volatility swaps and options on swaps. The swaps are defined via contingent claims whose payoffs depend on the terminal level of a discretely monitored version of the quadratic variation of some observable reference process. As such a process we consider a class of Levy models with stochastic time change. Our analysis reveals a natural small parameter of the problem which allows a general asymptotic method to be developed in order to obtain a closed-form expression for the fair price of the above products. As examples, we consider the CIR clock change, general affine models of activity rates and the 3/2 power clock change and give an analytical expression of the swap price. Comparison of the results obtained with a familiar log-contract approach is provided.

Using pseudo-parabolic and fractional equations for option pricing in jump diffusion models.

A. Itkin, P. Carr

Computational Economics, 2012, Vol 40, N.1, p.63-104

In mathematical finance a popular approach for pricing options under some Levy model is to consider underlying that follows a Poisson jump diffusion process. As it is well known this results in a partial integro-differential equation (PIDE) that usually does not allow an analytical solution while numerical solution brings some problems. In this paper we elaborate a new approach on how to transform the PIDE to some class of so-called pseudo-parabolic equations which are known in mathematics but are relatively new for mathematical finance. As an example we discuss several jump-diffusion models which Levy measure allows such a transformation.

Jumps without Tears: A New Splitting Technology for Barrier Options

A. Itkin, P. Carr

Int. Journal Numerical Analysis & Modeling, 2011, v.8, N.4, pp 667–704.

The market pricing of OTC FX options displays both stochastic volatility and stochastic skewness in the risk-neutral distribution governing currency returns. To capture this unique phenomenon Carr and Wu developed a model (SSM) with three dynamical state variables. They then used Fourier methods to value simple European-style options. However, pricing exotic options requires numerical solution of 3D unsteady PIDE with mixed derivatives which is expensive. In this paper to achieve this goal we propose a new splitting technique. Being combined with another method of the authors, which uses pseudo-parabolic PDE instead of PIDE, this reduces the original 3D unsteady problem to a set of 1D unsteady PDEs, thus allowing a significant computational speedup. We demonstrate this technique for single and double barrier options priced using the SSM.

New solvable stochastic volatility models for pricing volatility derivatives

A. Itkin

Review of Derivatives Research, 2013, v.16, #2, pp.111-134

Classical solvable stochastic volatility models (SVM) use a CEV process for instantaneous variance where the CEV parameter γ takes just few values: 0 - the Ornstein-Uhlenbeck process, 1/2 - the Heston (or square root) process, 1- GARCH, and 3/2 - the 3/2 model. Some other models were discovered in \cite{Labordere2009} by making connection between stochastic volatility and solvable diffusion processes in quantum mechanics. In particular, he used to build a bridge between solvable (super)potentials (the Natanzon (super)potentials, which allow reduction of a Schr\"{o}dinger equation to a Gauss confluent hypergeometric equation) and existing SVM. In this paper we discuss another approach to extend the class of solvable SVM in terms of hypergeometric functions. Thus obtained new models could be useful for pricing volatility derivatives (variance and volatility swaps, moment swaps).

Pricing options on illiquid assets with liquid proxies using utility indifference and dynamic-static hedging

I. Halperin, A. Itkin

Quantitative Finance, 2014, v.14, # 3, pp.427-442

This work addresses the problem of optimal pricing and hedging of a European option on an illiquid asset Z using two proxies: a liquid asset S and a liquid European option on another liquid asset Y. We assume that the S-hedge is dynamic while the Y-hedge is static. Using the indifference pricing approach, we derive a HJB equation for the value function, and solve it analytically (in quadratures) using an asymptotic expansion around the limit of the perfect correlation between assets Y and Z. While in this paper we apply our

framework to an incomplete market version of the credit-equity Merton's model, the same approach can be used for other asset classes (equity, commodity, FX, etc.), e.g. for pricing and hedging options with illiquid strikes or illiquid exotic options.

Pricing Illiquid Options with N+1 Liquid Proxies Using Mixed Dynamic-Static Hedging

I. Halperin, A. Itkin

International Journal of Theoretical and Applied Finance, 2013, vol.16, #7, pp.1350033-1 - 1350033-17.

We study a problem of optimal pricing and hedging of a European option written on an illiquid asset Z using a set of proxies: a liquid asset S, and N liquid European options P_i, each written on a liquid asset Y_i, i=1,N. We assume that the S-hedge is dynamic while the multi-name Y-hedge is static. Using the indifference pricing approach with an exponential utility, we derive a HJB equation for the value function, and build an efficient numerical algorithm. The latter is based on several changes of variables, a splitting scheme, and a set of Fast Gauss Transforms (FGT), which turns out to be more efficient in terms of complexity and lower local space error than a finite-difference method. While in this paper we apply our framework to an incomplete market version of the credit-equity Merton's model, the same approach can be used for other asset classes (equity, commodity, FX, etc.), e.g. for pricing and hedging options with illiquid strikes or illiquid exotic options.

Efficient Solution of Backward Jump-Diffusion PIDEs with Splitting and Matrix Exponentials.

A. Itkin

Journal of Computational Finance, 2016, v.19, pp. 29-70.

We propose a new, unified approach to solving jump-diffusion partial integro-differential equations (PIDEs) that often appear in mathematical finance. Our method consists of the following steps. First, a second-order operator splitting on financial processes (diffusion and jumps) is applied to these PIDEs. To solve the diffusion equation, we use standard finite-difference methods, which for multi-dimensional problems could also include splitting on various dimensions. For the jump part, we transform the jump integral into a pseudo-differential operator. Then for various jump models we show how to construct an appropriate first and second order approximation on a grid which supersets the grid that we used for the diffusion part. These approximations make the scheme to be unconditionally stable in time and preserve positivity of the solution which is computed via a matrix exponential. The paper demonstrates that the proposed method is computationally efficient, accurate and simple to implement.

Multimodal Transportation Network Modeling

by Hai Yang, Member EUAS

Short Biography

Prof. Hai Yang is currently a Chair Professor at The Hong Kong University of Science and Technology. He is internationally known as an active scholar in the field of transportation, with more than 240 papers published in SCI/SSCI indexed journals and a SCI H-index citation rate of 52. Most of his publications appeared in leading international journals, such as Transportation Research, Transportation Science and Operations Research. Prof. Yang received a number of national and international awards, including National Natural Science Award bestowed by the State Council of PR China (2011). He was appointed as Chang Jiang Chair Professor of the Ministry of Education of PR China; Prof. Yang served as the Editor-in-Chief of Transportation Research Part B: Methodological from 2013 to 2018 and is now a distinguished editorial board member of this journal.

Prof. Hai Yang's research record, seminal contributions and achievements are extraordinary. His contributions in the areas of transportation include: 1) 71 publications in Transportation Research Part B: Methodological, the most influential journal in the transportation field 2) 242 publications in SCI/SSCI-indexed journals, with an SCI H-index citation rate of 50 3) A total number of Google Scholar Citations 17979 and an H-index 70 (as of 23 October 2018). Some of his papers are among most highly cited articles in transportation. After persistent hard work and significant contributions to advancing the knowledge and understanding of transportation systems for twenty five years, Prof. Yang has established himself as a world leader in transportation research, his stature and authority in the international community of scholars is amply demonstrated by the fact—Prof Yang served as the third Editor-in-Chief (EiC) of Transportation Research Part B: Methodological (TR Part B), after Frank A Haight (1967-2003) and Fred L Mannering (2004-2012)—one of the highest recognitions by scholars in the broad field of transportation. As remarked by the executive publisher of Elservier, Chris Pringle, in an e-mail to the TR Part B editorial team: "Professor Yang has been highly successful as EiC of TR Part B by every key measure. Since his editorship from January 2013, the journal has doubled in size, both in terms of submissions (over 1,000 in 2017) and of accepted papers (now over 200 a year). Professor Yang has operated a highly efficient editorial process to handle this surge, and has maintained TR Part B's reputation as the premier methodological journal in its field, being consistently ranked at or close to #1 in its category, and currently with an impressive Impact Factor of 4.081."

He was one of the five world-renowned transportation scientists invited by the Beijing Municipal Commission of Transport for a real-time broadcast public forum on "Global Mega City Traffic Congestion Control" on 30 November 2017 (together with, Prof. Carlos Daganzo, Professor of UC Berkeley and Member of US National Academy of Engineering, Prof. Pravin Varaiya, Professor of UC Berkeley and Member of US National Academy of Engineering and US National Academy of Sciences, and Prof, Michael Walton, Professor of UT Austin and US National Academy of Engineering).

National and international recognition with awards and honors, among others

- *Chang Jiang Chair Professor of the Ministry of Education of PR China (Host University: Beijing University of Aeronautics and Astronautics).*
- *Guest Chair Professor of Tsinghua University and Beijing Jiao Tong University.*
- *Member of EU Academy of Sciences (offered in January 2018).*
- *The most cited researcher in the world (150 in total in civil engineering (from 2016 Academic Ranking of World Universities (ARWU) by academic subjects.*
- *Recipient of the 2012 HKUST Engineering Research Excellence*

- *Recipient of the esteemed 2011 Second-class National Natural Science Award of the PR China (the highest national award in science & engineering).*
- *37 invited keynote/plenary speeches in international conferences.*

Statement of Distinctive Academic Contributions

Professor Hai Yang is internationally known as a leading scholar in the field of transportation. He has distinguished himself through outstanding research at the forefront of analysis, modeling and optimization of transportation systems for more than twenty five years. In particular, he enjoys an excellent international reputation for his pivotal contributions to the following two key areas.

1. Multimodal transportation network modeling

Prof. Hai Yang has made distinguished contributions in the area of control and management of traffic congestion in general multimodal networks. He has achieved great success in dealing with network traffic flow problems by combining operational research methods and economic theory. The prominent originality of his achievements is particularly witnessed in opening to the transportation field new methodologies for transportation analysis. He was among the first to develop bi-level programming methods for a wide spectrum of critical transportation problems, such as network design, congestion pricing and traffic control. His pioneering work has sparked off development of a substantial stream of research in this area over the past fifteen years. In particular, Prof. Yang proposed innovative congestion pricing methodologies for reducing both traffic congestion and emissions on networks. More recently, Prof. Yang, together with his PhD students, has developed a novel mathematical and economic model that formalizes the analysis and application of a tradable travel credit scheme for network mobility management, in an efficient, flexible and equitable manner. His idea of a tradable credit scheme makes no one worse off and some better off in tackling urban traffic congestion, and has made tremendous impacts in the transportation research community. This ground-breaking scheme offers a unique and appealing solution towards developing an environmentally sustainable transportation system, which is widely regarded as one of the top priorities on current political agenda worldwide.

2. Economic analysis and modeling of on-demand transportation services

Prof. Hai Yang is a highly reputable researcher on the economic analysis and modeling of smart mobility. With his solid background in both microeconomics and operations research, Prof. Yang, together with his research students, developed a substantial stream of research on taxi service modeling. They successfully introduced the network equilibrium concept, traffic congestion effects, multi-period dynamic taxi services with endogenous service intensity, and bilateral taxi-customer searching and meeting, into the analysis and modeling of urban taxi services.

Indeed, Prof. Yang's skillful treatment of real world taxi industries has proven to be a remarkable advance over the large body of early research carried out by economists using aggregate and abstract analytical models, and moved the field a long way forward in terms of the scope of application of taxi models. His research in this area has been successfully applied to the Hong Kong taxi industry, where both occupied and vacant taxi movements constitute almost 25% of the overall traffic stream. Their analysis of nonlinear pricing of taxi services with Hong Kong data offered strong support for the Hong Kong SAR Government's implementation of a nonlinear fare structure for taxi services, a fare structure that raised short-haul fares and lowered long-haul fares.

Prof. Yang's pioneering work on network modeling of urban taxi services offered a precise understanding of the equilibrium nature of taxi services. His seminal and unique contributions subsequently and substantially influenced and greatly shaped the fundamental theory for the current analysis of emerging on-demand ride services. The current on-demand ride-sharing platforms offer benefits for individual users such as cost savings and for the society such as alleviating traffic congestion and reducing emissions, and are now receiving increasing attention worldwide. It is anticipated that the basic theory of taxi industry developed by Prof. Yang will also become the foundation for developing and implementing smart mobility in our future cities when ride-sharing with autonomous cars becomes a market reality.

Automatic Facial Expression Learning Method based on Humanoid Robot XIN-REN

by Fuji Ren, Member EUAS

Short Biography

Prof. Fuji Ren received his B.E. and M.E. degrees from Beijing University of Posts and Telecommunications, Beijing, China, in 1982 and 1985, respectively. He received his Ph.D. degree in 1991 from Hokkaido University, Japan. He is a professor in the Faculty of Engineering of Tokushima University, Japan. His research interests include information science, artificial intelligence, language understanding and communication, affective computing, and Intelligent robot. He is a member of The Engineering Academy of Japan, a fellow of IEICE and CAAI. He is a fellow member of the Japan Federation of Engineering Societies. He is the president of the International Advanced Information Institute. He is the author/co-author/editor of eight books and over 500 research publications.

Automatic Facial Expression Learning Method based on Humanoid Robot XIN-REN

Fuji Ren and Zhong Huang

IEEE TRANSACTIONS ON HUMAN-MACHINE SYSTEMS, VOL. 46, NO. 6, DECEMBER 2016, 810 – 821.

Abstract

The ability of a humanoid robot to display facial expressions is an essential factor for a natural human–computer interaction. An automatic facial expression learning method under the kinematic constraints of the humanoid robot XIN-REN is proposed to generate human-like and less hardwired robot facial expressions. First, the forward kinematics model, which is designed to reflect the nonlinear mapping relationship between the servo displacement vector and its corresponding expression shape vector, is converted into the linear relationship between the mechanical energy of the servo displacements and the potential energy of the feature points based on the energy conservation principle. Second, the improved inverse kinematics model, which is under the constraints of instantaneous similarity

and movement smoothness, is established and solved by the exterior point penalty function method. Finally, an online expression learning is employed to determine the optimal servo displacements for transferring the facial expression of the human performer to the robot based on the inverse kinematics model. To illustrate the performance of the proposed method, we conduct the evaluation experiments for the forward kinematics models and inverse kinematics models based on the collected data from the robot's random states as well as fixed procedure by animators. Meanwhile, according to three sequential indicators (space-similarity, time-similarity, and movement smoothness), we further evaluate the facial imitation ability with different values of weighting factor. The experimental results indicate that the mean shape deviation and position deviation does not exceed 6 pixels and 3 pixels, and the average servo displacement deviation does not exceed 0.8%. Compared with related works, the proposed system provides a better space–time similarity to the performer and maintains a smoother trajectory for multi-frame sequential imitation.

Facial Expression Recognition based on Multi-regional D-S Evidences Theory Fusion

Fuji Ren

IEEJ Transactions on Electrical and Electronic Engineering 12(2), December 2016, p.p. 251 – 261.

To achieve decision-level fusion of the multi-regional features and highlight the credibility of different regional evidences, a facial expression recognition method based on multi-regional evidences fusion is proposed. The block histogram of gradient Gabor features in three regions such as eyebrows, eyes and mouth, are extracted from facial image and are taken as evidences of expression classification. Then, the category-membership and regional-contribution are solved by using region weighted semi-supervised Fuzzy c-means clustering (FCM) algorithm for constructing initial basic probability assignment (BPA) and emphasizing the different importance of evidences, respectively. Moreover, the initial BPA of evidences are further reassigned by combining the region-contribution and evidence-supportability for reducing evidential conflict. Finally, the final decision-level fusion of multi-regional evidences is obtained based on Dempster-Shafer combination rule. The experimental results on Cohn-Kanade expression database show that the BPA construction method based on category-membership degree and the reassignment strategy based on region-contribution and evidence-supportability improve the recognition rate and keep good robustness for all kind of expressions. Meanwhile, compared with existing decision-level fusion strategies and classification methods, the proposed recognition framework based on D-S evidences theory has advantages in recognition performance and reliability, especially increases recognition rate for expressions which are hard to distinguish, such as fear, sadness and disgust.

The Complexity of the Pathogenesis of Psoriasis

by Peter van de Kerkhof, Member EUAS

Short Biography

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Peter CM van de Kerkhof is emeritus Professor of Dermatology and immediate past chairman of the department of Dermatology of Radboud University Nijmegen. He is currently the coordinating Medical Officer of the International Psoriasis Council and chair of the scientific advisory board of the dutch burn association. He has been working for many years on the pathogenesis and treatment of psoriasis. He has published more than 700 publications in peer reviewed journals and has given many presentations on invitation at international conferences.
He has served as president of the ESDR and EDF and was board member of various international societies. He is the past---president of the International Psoriasis Council.
Current interests are:
Pathogenesis and development of biomarkers for psoriasis
Real clinical practise research
Personalised medicine

Psoriasis is a common hereditary skin disease which is characterised by sharply defined, red, scaly plaques. On a microlevel, this corresponds to an inflammation and a thickened, incompletely keratinizing epidermis (1). As the result of an exceptionally strong immune system, a new psoriasis lesion occurs at sites of injury to the skin. On the other hand, psoriasis is a disease of the entire body with symptoms such as joint inflammations or overweight and diabetes or cardiovascular disease. Treatment involves a simple, external therapy with a corticosteroid or vitamin D derivate as a first step and, in case of insufficient improvement, phototherapy or systemic treatment with fumarate, methotrexate, cyclosporine, acitretin, apremilast or one of the biologics, targeted at TNF alpha, IL-17 or IL-23. These approaches comprehend a wide range of therapies, making it possible to find the most effective treatment for each patient.

In the 1970s, psoriasis was considered a disorder of the epidermis. In our research group, an increased recruitment of proliferating cells from the non-proliferating G0 compartment was found in the psoriasis plaque 2)): a universal mechanism of recovery of the epidermis which was not disease-specific.

Micropustules of neutrophilic granulocytes in the epidermis are typical of psoriasis. During flare-ups, the density of these micropustules is high (3,4), decreasing sharply afterwards. Neutrophilic granulocytes are part of the innate immune system. By contrast,

the density of the inflammatory cells belonging to adaptive immunity (including CD45 RO + cells and Th1 cells) increases in the course of the disease process (5). However, these inflammatory cells are not organised as micropustules. So the spatial organisation of the cellular components of innate and adaptive immunity are completely different. But both systems also have different dynamics. Our research showed that innate cellular immunity is dominant in the acute lesion while in the chronic lesion, cellular adaptive immunity is dominant.

But what about the molecular aspect? In the 1980s, Schalkwijk et al discovered that patients with psoriasis produce proteins in the epidermis which are highly relevant for the innate immune system. Research into 'skin derived anti-leukoproteinase' (6) and, later, into the 'beta defensins' (7) and the very special discovery of an increased 'beta-defensin genomic copy number' (8) indicate a dominance of innate immunity in patients with psoriasis at the molecular level. Furthermore, an increased production of the cytokines TNF alpha, IL-17, and Il-23, also part of innate immunity, was observed (9-11).

Keijser et al demonstrated that IL-17 is mainly produced by neutrophilic granulocytes in the psoriatic lesion (12). Treatments targeted at TNF alpha, IL-17 and IL-23 appear to be very effective and safe for patients with psoriasis, which strongly supports the relevance of innate immunity in the pathogenesis of psoriasis.

A persistent clonality of T-cells in patients with psoriasis was demonstrated by Prinz et al , which indicates that certain T-cells are selected in the adaptive immunity. According to the original concept, IL-17 is selectively produced by Th-17 cells and because of that, it would be a cytokine of the adaptive immunity (13). However, IL-17 has a dual origin produced by the neutrophilic granulocytes of innate immunity and by Th17 cells of adaptive immunity, amongst other cells.

How is adaptive immunity distributed over the chronic psoriasis plaques? In patients with chronic stable psoriasis, a heterogeneous division of blood perfusion was found despite a uniform erythema: 'hot spots' of perfusion pulsating synchronically with the heartbeat. While there is not a single change of the erythema in these plaques as observed by the human eye, the pattern of hot spots of perfusion shows dynamic change over time. Within these hot spots we observed an increased density of Th1 cells (cells of adaptive immunity) and an increased transcription and protein expression of IL-17 (14). With the human eye, a uniform static redness of the psoriasis plaques was observed. The dynamic multifocal organisation of adaptive immunity could be imaged by 'laser doppler perfusion imaging'. In addition to the Th17 cell, other inflammatory cells also start to produce IL-17 in the chronic phase of the psoriasis plaques. For example, it has been demonstrated that Fox p3+regulatory T cells can differentiate to IL-17 producing cells (15).

Several genes have been identified as 'psoriasis susceptibility genes', genes that are involved in innate immunity as well as in adaptive immunity (1). But genetic changes in relation to differentiation of the epidermis also appear to be associated with psoriasis. For example, deletions of LCE3 genes form an important risk factor for developing psoriasis (16). Genes from various biological systems contribute to the development of psoriasis. Each patient with psoriasis seems to have his own set of psoriasis genes. Hence psoriasis is a genetic disease linked to different biological systems, especially innate immunity, adaptive immunity and differentiation of the epidermis. From an evolutionary viewpoint, psoriasis has the advantage of an increased resistance against bacteria but the disadvantage of the itchy scaly skin disease and comorbidities such as arthritis, and an increased risk of diabetes and of cardiovascular disease.

Innate and adaptive immunity are 'branching immune pathways', branching inflammatory mechanisms with IL-17 and IL-23 being a connecting thread of both the

acute phase to the chronic phase of the psoriatic process. However, the composition of the cells that produce these cytokines, changes from a dominance of innate immunity in the acute phase to a dominance of adaptive immunity in the chronic phase.

Patients usually start with external therapy and, in case of insufficient results, this is followed by UVB treatment, classic systemic drugs and biologics. The treatment choice is highly individual, taking into account many patient characteristics and the type of skin disease. A broad range of treatments with, at present, 8 biologics offers the patient a real choice. One of the major research activities of the department is optimising the management of the individual patient's treatment. In our research we strive to find associations between the genetic constitution and course of disease .

In practice, the treatment of psoriasis is monitored by objective scores for disease severity such as Psoriasis Area Severity Index (PASI) and Body Surface Area (BSA). These classic disease severity scores do not reveal the actual disease activity. Only when the activity of the disease process has been incorporated in the disease severity scores, we will be able to find meaningful correlations between potential biomarkers and the clinic phenotypes and disease progress.

Pinpoint papules and expansion of lesions reflect the activity of the process. We can imagine the activity of the process in the perspective of immunity

1. Imaging the density of perfusion hot spots through laser doppler perfusion, correlating to foci of Th1 cells.
2. Imaging of micropustules of Kogoj through confocal in vivo microscopy, correlating to foci of neutrophilic granulocytes.
3. Quantifying of cytokine patterns in the psoriasis lesion.

Managing treatments on the basis of disease activity and biomarkers will help us find the right therapy for each patient in the future.

What is the course of skin diseases in connection with triggering factors and other diseases, the comorbidities? I will again restrict myself to psoriasis.

Triggers such as psychological stress, medications and focal infections may worsen symptoms of psoriasis. Well-known comorbidities are joint inflammation, diabetes and cardiovascular disease. Clinical practice gives the impression that there are far more triggering factors and comorbidities, an impression that is ,however, not evidence-based. Of course, this does not mean that such connections have no relevance for the individual patient. Which triggering factors are relevant for a certain patient and which patient will develop certain comorbidities remains hidden.

Over the years, a wealth of research data has been generated on heredity, pathogenesis, epidemiology, quality of life, comorbidities and response to psoriasis treatments. An important development are the evidence based guidelines. Guideline development is performed by working parties of dermatologists, working together on an ever improving system of guidelines. The classic 'evidence-based' research has the well-known limitation of the small number of variables per study. This reductionist approach to research does not show what is most important for the individual patient in practice: giving meaning to a range of triggering factors and the risk management of comorbidities. Medicine requires integrative evidence.

In practice, how do we take the right decision for the individual patient if the evidence cannot be provided? The patient needs a good doctor who pays attention to triggering factors that are often hidden. He listens to the patient, examines the patient and discovers the things that are hidden. He then makes a diagnosis and provides personalised care and support. The good doctor is scientifically trained and permanently educated. He knows the

important values but also the restrictions of the 'evidence' of the treatments. The good doctor is 'self-learning', constantly fed by his experiences with individual patients and capable of integrating these experiences. He is an empathic and systematic thinker. He instinctively knows how to get to the essence which lies buried under the multitude of triggering factors. He will offer his patient the care that is needed in his specific situation. Medicine is the art of patient care. Quoting Paul Klee: 'Art does not reflect what is seen, rather it makes the hidden visible.'

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Contributions in Head and Neck Cancer of Clinical and Translational Research

by Dong Moon Shin, Member EUAS

Short Biography

Dong Moon Shin, MD, FACP, FAAAS
Professor of Medical Oncology and Francis Kelly Blomeyer Chair in Cancer Research
Emory University School of Medicine

Dr. Dong Moon Shin is currently Professor of Medical Oncology, Otolaryngology and Biomedical Engineering, and holds Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research in the Department of Hematology and Medical Oncology at Winship Cancer Institute of Emory University. He graduated from Yonsei University College of Medicine and trained for Residency in Internal Medicine at Cook County Hospital, Chicago, IL and Medical Oncology at the University of Texas M. D. Anderson Cancer Center, Houston, TX. He has served as a faculty member in the Department of Thoracic/Head and Neck Medical Oncology at M. D. Anderson Cancer Center and University of Pittsburgh as Professor and Director of Head and Neck Cancer Program before he joined Emory University.

Honors and Awards

2018- Present Member of the EU Academy of Sciences (EUAS)
2017 Best Doctors in America (Oncology) (2003-2017)
2016 Top Doctors (Oncology) in Atlanta Magazine (Consecutively for 11 years)
2016 Member of the "Millipub" club (2,000 citations) of the Emory UniversitySchool of Medicine {NEJM 354: 567-78, 2006.}
2016 Elected Fellow of American Association of the Advancement of Science(FAAAS)
2015 Member of the "Millipub" club (2 articles cited more than 1000 times) of the Emory University School of Medicine {Nature Biotech. 26(1):83-90,
2008; Nature Rev. Drug Discovery. 7:771-82, 2008.}
2015 The 18th KBS (Korean Broadcasting System) Global Korean Award: Science and Technology
2014 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd. (Consecutively for 8 years)
2013/2012 Top Doctors featured in U.S. News & World Report
2011 Member of "Millipub" (article cited more than 1000 times) club of the Emory University School of Medicine {NEJM. 345:567-578, 2006.}
2010 Top Doctors (Oncology) in Atlanta Magazine
2010 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd.
2009 (Oct.) Honorary Professor at Central South University, Changsha, China
2009 Americas Top Doctors in Cancer by Castle Connolly Medical, Ltd
2009 Best Doctors in America (Oncology)
2009 Top Doctors (Oncology) in Atlanta Magazine
2009 Awardee of the Grand Prize for Medical Science in 2009 by Yonsei University, Seoul, Korea
2008 Top Doctors (Oncology) in Atlanta Magazine
2008 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd.
2008 Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research
2007 Cambridge Who's Who Life Time Member
2007 America's Top Oncologists by Consumers' Research Council of America
2005 Best Doctors in America (Oncology)
2005 Georgia Cancer Coalition (GCC) Distinguished Scholar Award

2005 Top Doctors (Oncology) in Atlanta
2004 Best Doctors in America
2003 Best Doctors in America
2001 Doris Duke Distinguished Clinical Scientist Award Nominee, Universityof Pittsburgh
2000 Faculty Scholar Award Nominee, M. D. Anderson Cancer Center
1994 Marquis Who's Who in the South and Southwest
1994 Distinguished Leadership Award for Cancer Research, American Biographical Institute, Inc.
1992 Fellowship of American College of Physicians
1994 Recipient of Clinical Oncology Career Development Award, American Cancer Society
1989 Who's Who in Medical Specialty
1987 Award of University Cancer Foundation (UCF) Research Funds

Dr. Shin is a renowned medical oncologist and prominent physician-scientist recognized for his work in the field of head and neck cancer of clinical and translational research. He has extensive experiences in the design and conduct of phase I-III clinical trials. Particularly, Dr. Shin has developed several important therapeutic regimens for treatment of cancer and the following examples are highlighted. He has developed combinations of paclitaxel, ifosphamide and cisplatin (TIP) and paclitaxel, ifosphamide and carboplatin (TIC) for metastatic squamous cell carcinoma of the head and neck (SCCHN) in 1990s. At around the same time he had also conducted an important clinical trial using combination of cyclophosphamide, doxorubicin, cisplatin and prednisone (CAPPr) for recurrent thymic carcinoma and the same CAPPr regimen was also developed as one of the induction regimens for locally advanced malignant thymoma. Such chemotherapeutic regimen is still being using in the oncology community as one of the standard chemotherapeutic regimens for thymic carcinoma or malignant thymoma. Dr. Shin's translational research interests includes chemoprevention, biochemoprevention, biomarker studies in head and neck cancer, nanotherapeutics for drug delivery, and other biomedical research for novel technology development.

Over the last 30 years Dr. Shin has extensively studied carcinogenesis, molecular-driven preclinical and clinical chemoprevention or biochemoprevention studies using synthetic retinoids and interferon-alpha and alpha-tocopherol in SCCHN. These studies including preclinical and phase I/II clinical studies to block the carcinogenesis process of the head and neck, and eventually prevent invasive cancers. Further, the studies have expanded to combination of EGFR-TKIs (i.e., erlotinib) and Cox-2 inhibitors (i.e., celecoxib) in the pre-clinical model and showed that the combination was highly synergistic to suppress oral carcinogenesis. And the combination has been conducted in the clinical trials and showed excellence pathologic responses in the advanced premalignant lesions of the oral cavity and larynx. Dr. Shin and his colleagues have further expanded the chemoprevention studies to the natural compounds, including green tea polyphenols (PPE), resveratrol, luteolin (from green vegetable) and honokiol (from magnolia extract) in preclinical studies. In particular, the combination of green tea PPE and EGFR-TKI (i.e., erlotinib) has an excellent synergistic effects in preclinical studies including xenograft animal models and better toxicity profile. And his team have recently conducted phase 1b study for the patients with advanced premalignant lesions (mild, moderate, severe dysplasia and carcinoma in situ) of the oral cavity and larynx. The abstract has been submitted to the 2019 annual meeting of the American Society of Clinical Oncology (ASCO).

Further, Dr. Shin has been also devoted for development of EGFR targeted therapy for SCCHN. He initiated a seminal phase 1 study of C225 (it was named later as

cetuximab) in combination with cisplatin in recurrent and metastatic head and neck cancer, and it was an important base of EGFR driven targeted therapy. Right after the phase 1 trial, an important multi-institutional phase III clinical trial was conducted by combining cetuximab with radiation therapy vs. radiation alone for locally advanced SCCHN, and the combination with radiation therapy arm showed a significant survival benefit compared to the radiation alone, and cetuximab was approved by the U.S. F.D.A. in 2006 for indication of therapy of SCCHN.

Dr. Shin's research has been well funded through funding from NIH/NCI (R01s, U01s, R21, etc.) and other funding agencies. Specifically he has been Principal Investigator of Emory University's Head and Neck Cancer SPORE program (***S***pecialized ***P***rograms ***of R***esearch ***E***xcellence), which was awarded to Emory in 2007 by the National Cancer Institute (NCI). Another area of his interest has been nanotechnology based anti-cancer drug delivery in collaboration with several other investigators including biomedical engineers, chemists, material scientists, imaging experts and animal scientists. The team has successfully developed biodegradable therapeutic nanoparticles to smartly deliver taxanes and cisplatin to xenografted tumors in vivo studies. More recently Dr. Shin in collaboration with biomedical engineers has studied gold nanoparticles by using photothermal therapy in animal models and showed a promising and effective anti-cancer activities. DNA nanoparticles as delivery vehicles have been applied for si-RNA molecules of certain genes or other therapeutic agents for cancer therapy. Dr. Shin has been collaborated with biomedical engineers to delivery such anti-cancer agents (including siRNA of Bcl2) to the tumor bearing animal models. Although the studies are still in the early stages of development, such smart delivery of the anticancer drugs is a highly promising field in order to improve efficacy of the drugs while toxicity induced by the drugs can be minimized or eliminated.

Dr. Shin has received many awards including the Best Doctors in America since first selected in 2003, Top Doctors (Oncology) in Atlanta Magazine and America's Top Doctors in Cancer (by Castle Connolly Medical Ltd.) since 2005, Distinguished Leadership Award for Cancer Research from American Biographical Institute, Georgia Cancer Coalition Distinguished Scholar Award, the 2009 Yonsei University's Medicine Grand Prize Award, Honorary Professor at Central South University, China, the Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research, and the 18th KBS Global Korean Award (in the category of Science and Technology). And he was also bestowed for Fellow of American Association of Advancement of Science (FAAAS) and many others.

Dr. Shin has also chaired numerous peer-review committees, including but not limited to the American Head and Neck Society, American Association of Cancer Research and the American Society of Clinical Oncology. He has also served as a member of many study sections at the National Cancer Institute, NIH and on the editorial boards (more than 15 scientific journals) including the Journal of Clinical Oncology, Clinical Cancer Research, Cancer Prevention Research, Molecular Cancer Therapeutics, International Journal of Oncology and others. He has published more than 340 articles in peer-reviewed journals (H-index of 68 and more than 25,000 citation numbers as of January 2019) in addition to more than 350 other publications including meeting abstracts, books, book chapters and monographs.

In Search of a Therapy for Alzheimer's Disease

by George Perry, Member EUAS

Short Biography

George Perry is dean of the College of Sciences, professor of biology and chemistry, and holds the Semmes Foundation Distinguished University Chair in Neurobiology at The University of Texas at San Antonio. Perry is recognized in the field of Alzheimer's disease research, particularly for his work on oxidative stress.

Perry received his Bachelor of Arts degree in zoology with high honors from University of California, Santa Barbara. After graduation, he headed to Scripps Institution of Oceanography, Hopkins Marine Station and Woods Hole, and obtained his Ph.D. in marine biology. He then received a postdoctoral fellowship in the Department of Cell Biology in the laboratories of Drs. Bill Brinkley and Joseph Bryan at Baylor College of Medicine, where he laid the foundation for his observations of abnormalities in cell structures.

In 1982 Perry joined the faculty of Case Western Reserve University, where he currently holds an adjunct appointment. He is distinguished as one of the top Alzheimer's disease (AD) researcher with over 1,000 publications, one of the top 100 most-cited scientists in neuroscience and behavior, and one of the top 25 scientists in free radical research. Perry has been cited over 77,000 times (H=140) and is recognized as an ISI highly cited researcher.

For nearly four decades of our research has focused on dissecting the cytopathology of Alzheimer's disease (AD) with the goal of developing a cure. We have used oxidative stress as a window to view and understand AD. Oxidative damage to sugars, proteins, lipids and nucleic acids is increased in neuronal cytoplasm. The same neuronal compartment has increased redox-active iron and copper, that can catalyze oxidative damage, that likely derive from mitochondrial debris (in and outside lysosomes) including cytochromes, mitochondria specific prosthetic groups and mtDNA. Mitochondria show altered axonal transport, size distribution, energetics, fusion/fission, and degradation in AD that correlate with the extent of oxidative damage suggesting they are the origin. Surprisingly, amyloidβ and tau are quantitatively associated with reduced neuronal oxidative damage. Copper sequestration by amyloidβ blocks copper mediated oxidation of lipids and vitamin C indicating amyloidβcan be a protective

response rather than the initiator of AD. Instead of being bound to amyloidβ, iron is present as 10nm magnetite crystals with super paramagnetic properties. Not just amyloidβ, but also tau, stress responses and activation of glutathione production are protective responses induced in AD to maintain neurons with altered balance for decades. While these studies put oxidative stress at the center of AD, they also highlight a complexity of multifaceted alterations that is homeostatic and requires a deeper level of understanding before an effective therapy or cure can be found.

Characterization of Proteins Present in Isolated Senile Plaques from Alzheimer's Diseased Brains by MALDI-TOF MS with MS/MS

Kelley, Andrea R., Perry, George, Bach, Stephan B. H.

ACS CHEMICAL NEUROSCIENCE, 9(2018), 708-714

Abstract

The increase of insoluble senile plaques in the brain is a primary hallmark of Alzheimer's disease. The usefulness of matrix-assisted laser desorption/ionization time of-flight mass spectrometry (MALDI-TOF MS) with tandem MS for the characterization of senile plaques from AD brains and the relevance of the components identified to furthering AD research using MS is discussed. Thirty-three components were reproducibly observed within tryptic aliquots of senile plaques from two different AD brains after sample preparation optimization. Additionally, this is one of the first accounts of LIFT being utilized for the direct sequencing of peptides from isolated senile plaques. While many of the species observed coisolated within senile plaques have been linked to AD etiology, if only speculatively, this is the first instance that many of them have been demonstrated to be a part of the plaques themselves. This work is the first step in determining the potential roles that the species may have in the aggregation or proliferation of the plaques.

Diminished O-GlcNAcylation in Alzheimer's disease is strongly correlated with mitochondrial anomalies.

Pinho Tiffany S, Correia Sonia C, Perry George, Ambrosio Antonio Francisco Moreira Paula

Biochimica et biophysica acta. Molecular basis of disease, 2018

Abstract

Uncover the initial cause(s) underlying Alzheimer's disease (AD) pathology is imperative for the development of new therapeutic interventions to counteract AD-related symptomatology and neuropathology in a timely manner. The early stages of AD are characterized by a brain hypometabolic state as denoted by faulty glucose uptake and utilization and abnormal mitochondrial function and distribution which, ultimately, culminates in synaptic "starvation" and neuronal degeneration. Importantly, it was recently recognized that the post-translational modification beta-N-acetylglucosamine (O-GlcNAc)

modulates mitochondrial function, motility and distribution being proposed to act as a nutrient sensor that links glucose and the metabolic status to neuronal function. Using post-mortem human brain tissue, brain samples from the triple transgenic mouse model of AD (3xTg-AD) and in vitro models of AD (differentiated SH-SY5Y cells exposed to AD-mimicking conditions), the present study is aimed to clarify whether O-GlcNAcylation, the posttranslational modification of intracellular proteins by O-GlcNAc, contributes to "mitochondrial pathology" in AD and its potential as a therapeutic target. A reduction in global O-GlcNAcylation levels was observed in the brain cortex and hippocampus of AD subjects. Moreover, GlcNAcylation levels are higher in mature mice but the levels of this posttranslational modification are lower in 3xTg-AD mice when compared to control mice. The in vitro models of AD also exhibited a marked reduction in global O-GlcNAcylation levels, which was strongly correlated with hampered mitochondrial bioenergetic function, disruption of the mitochondrial network and loss of cell viability. Conversely, the pharmacological modulation of O-GlcNAcylation levels with Thiamet-G restored O-GlcNAcylation levels and cell viability in the in vitro models of AD. Overall, these results suggest that O-GlcNAcylation is involved in AD pathology functioning as a potential link between mitochondrial energetic crisis and synaptic and neuronal degeneration. This posttranslational modification represents a promising therapeutic target to tackle this devastating neurodegenerative disease.

Towards an Integrative Understanding of tRNA Aminoacylation-Diet-Host-Gut Microbiome Interactions in Neurodegeneration

Paley Elena L., Perry George

NUTRIENTS, 10(2018)

Abstract

Transgenic mice used for Alzheimer's disease (AD) preclinical experiments do not recapitulate the human disease. In our models, the dietary tryptophan metabolite tryptamine produced by human gut microbiome induces tryptophanyl-tRNA synthetase (TrpRS) deficiency with consequent neurodegeneration in cells and mice. Dietary supplements, antibiotics and certain drugs increase tryptamine content in vivo. TrpRS catalyzes tryptophan attachment to tRNA t rP at initial step of protein biosynthesis. Tryptamine that easily crosses the blood-brain barrier induces vasculopathies, neurodegeneration and cell death via TrpRS competitive inhibition. TrpRS inhibitor tryptophanol produced by gut microbiome also induces neurodegeneration. TrpRS inhibition by tryptamine and its metabolites preventing tryptophan incorporation into proteins lead to protein biosynthesis impairment. Tryptophan, a least amino acid in food and proteins that cannot be synthesized by humans competes with frequent amino acids for the transport from blood to brain. Tryptophan is a vulnerable amino acid, which can be easily lost to protein biosynthesis. Some proteins marking neurodegenerative pathology, such as tau lack tryptophan. TrpRS exists in cytoplasmic (WARS) and mitochondrial (WARS2) forms. Pathogenic gene variants of both forms cause TrpRS deficiency with consequent intellectual and motor disabilities in humans. The diminished tryptophan-dependent protein biosynthesis in AD patients is a proof of our model-based disease concept.

Nanoscale synchrotron X-ray speciation of iron and calcium compounds in amyloid plaque cores from Alzheimer's disease subjects

Everett James, Collingwood Joanna, Tjendana-Tjhin, Vindy, Brooks Jake, Lermyte Frederik, Plascencia-Villa German, Hands-Portman, Ian, Dobson, Jon, Perry George, Telling Neil D.

NANOSCALE, 10(2018)

Abstract

Altered metabolism of biometals in the brain is a key feature of Alzheimer's disease, and biometal interactions with amyloid-ss are linked to amyloid plaque formation. Iron-rich aggregates, including evidence for the mixed-valence iron oxide magnetite, are associated with amyloid plaques. To test the hypothesis that increased chemical reduction of iron, as observed in vitro in the presence of aggregating amyloid-ss, may occur at sites of amyloid plaque formation in the human brain, the nanoscale distribution and physicochemical states of biometals, particularly iron, were characterised in isolated amyloid plaque cores from human Alzheimer's disease cases using synchrotron X-ray spectromicroscopy. In situ X-ray magnetic circular dichroism revealed the presence of magnetite: a finding supported by ptychographic observation of an iron oxide crystal with the morphology of biogenic magnetite. The exceptional sensitivity and specificity of X-ray spectromicroscopy, combining chemical and magnetic probes, allowed enhanced differentiation of the iron oxides phases present. This facilitated the discovery and speciation of ferrous-rich phases and lower oxidation state phases resembling zero-valent iron as well as magnetite. Sequestered calcium was discovered in two distinct mineral forms suggesting a dynamic process of amyloid plaque calcification in vivo. The range of iron oxidation states present and the direct observation of biogenic magnetite provide unparalleled support for the hypothesis that chemical reduction of iron arises in conjunction with the formation of amyloid plaques. These new findings raise challenging questions about the relative impacts of amyloid-ss aggregation, plaque formation, and disrupted metal homeostasis on the oxidative burden observed in Alzheimer's disease.

Mfn2 ablation causes an oxidative stress response and eventual neuronal death in the hippocampus and cortex

Jiang Sirui, Nandy Priya, Wang Wenzhang, Ma Xiaopin, Hsia Jeffrey, Wang Chunyu, Wang Zhenlian, Niu Mengyue, Siedlak, Sandra L., Torres, Sandy

MOLECULAR NEURODEGENERATION, 13(2018)

Abstract

Background: Mitochondria are the organelles responsible for energy metabolism and have a direct impact on neuronal function and survival. Mitochondrial abnormalities have been well characterized in Alzheimer Disease (AD). It is believed that mitochondrial fragmentation, due to impaired fission and fusion balance, likely causes mitochondrial dysfunction that underlies many aspects of neurodegenerative changes in AD.

Mitochondrial fission and fusion proteins play a major role in maintaining the health and function of these important organelles. Mitofusion 2 (Mfn2) is one such protein that regulates mitochondrial fusion in which mutations lead to the neurological disease.

Methods: To examine whether and how impaired mitochondrial fission/fusion balance causes neurodegeneration in AD, we developed a transgenic mouse model using the CAMKII promoter to knockout neuronal Mfn2 in the hippocampus and cortex, areas significantly affected in AD.

Results: Electron micrographs of neurons from these mice show swollen mitochondria with cristae damage and mitochondria membrane abnormalities. Over time the Mfn2 cKO model demonstrates a progression of neurodegeneration via mitochondrial morphological changes, oxidative stress response, inflammatory changes, and loss of MAP2 in dendrites, leading to severe and selective neuronal death. In this model, hippocampal CA1 neurons were affected earlier and resulted in nearly total loss, while in the cortex, progressive neuronal death was associated with decreased cortical size.

Conclusions: Overall, our findings indicate that impaired mitochondrial fission and fusion balance can cause many of the neurodegenerative changes and eventual neuron loss that characterize AD in the hippocampus and cortex which makes it a potential target for treatment strategies for AD

Mitofusin 2 Regulates Axonal Transport of Calpastatin to Prevent Neuromuscular Synaptic Elimination in Skeletal Muscles

Wang Luwen, Gao Ju, Liu Jingyi, Siedlak Sandra L., Torres, Sandy, Fujioka, Hisashi, Huntley Mikayla L., Jiang Yinfei, Ji Haiyan, Yan Tingxiang

CELL METABOLISM, 28(2018)

Abstract

Skeletal muscles undergo atrophy in response to diseases and aging. Here we report that mitofusin 2 (Mfn2) acts as a dominant suppressor of neuromuscular synaptic loss to preserve skeletal muscles. Mfn2 is reduced in spinal cords of transgenic SOD1 G93A and aged mice. Through preserving neuromuscular synapses, increasing neuronal Mfn2 prevents skeletal muscle wasting in both SOD1 G93A and aged mice, whereas deletion of neuronal Mfn2 produces neuromuscular synaptic dysfunction and skeletal muscle atrophy. Neuromuscular synaptic loss after sciatic nerve transection can also be alleviated by Mfn2. Mfn2 coexists with calpastatin largely in mitochondria-associated membranes (MAMs) to regulate its axonal transport. Genetic inactivation of calpastatin abolishes Mfn2-mediated protection of neuromuscular synapses. Our results suggest that, as a potential key component of a novel and heretofore unrecognized mechanism of cytoplasmic protein transport, Mfn2 may play a general role in preserving neuromuscular synapses and serve as a common therapeutic target for skeletal muscle atrophy.

Electrooxidation of Formic Acid Enhanced by Surfactant-Free Palladium Nanocubes on Surface Modified Graphene Catalyst

by Malcolm Green, Member EUAS

Short Biography

Name: *GREEN, Malcolm Leslie Hodder*
Address: *St Catherine's College, Oxford or*
Inorganic Chemistry Laboratory
South Parks Road
OXFORD, OX1 3QR
Date of Birth: *16/4/36, Eastleigh, Hampshire*
Nationality: *British*
Marital Status: *Married. Three children*
Degrees: *B.Sc.(Hons), London; D.I.C., M.A.(Cantab), M.A.(Oxon), C.Chem., F.R.S.C., Ph.D., F.R.S.*

ACADEMIC CAREER

1953-56 *Acton Technical College, University of London, B.Sc Hons. Chemistry*
1956-59 *Imperial College of Science and Technology, London; D.I.C. Ph.D. in chemistry. Supervisor Professor Sir G. Wilkinson*
1959-60 *Post-doctoral Research Associates Fellow. Imperial College of Science and Technology*
1960-63 *Assistant Lecturer in Inorganic Chemistry at Cambridge University*
1961 *Fellow of Corpus Christi College, Cambridge*
1963 *Septcentenary Fellow of Inorganic Chemistry, Balliol College, Oxford and Departmental Demonstrator, University of Oxford*
1965 *University Lecturer, University of Oxford*
1971 *Visiting Professor, University of Western Ontario (Spring Term)*
1972 *Visiting Professor, Ecole de Chimie and Institute des Substances Naturelles, Paris*
1973 *A.P. Sloan Visiting Professor, Harvard University*
1979-84 *Appointed to the British Gas Royal Society Senior Research Fellowship*
1981 *Sherman Fairchild Visiting Scholar at the California Institute of Technology*
1984. *Re-appointed British Gas Royal Society Senior Research Fellow (1984-6)*
1987 *Vice-master, Balliol College, Oxford*
1989 *Appointed Professor of Inorganic Chemistry and Head of Department, Oxford University Fellow of St Catherine's College, Oxford*
2004- present *Emeritus Research Professor in the Inorganic Chemistry Laboratory, Oxford Emeritus Fellow of Balliol College and St Catherine's College*

Publications *Two text books, 738 refereed papers and 8 patents.*

Honours

1974 *Corday-Morgan Medal and Prize in Inorganic Chemistry (Royal Society of Chemistry)*
1977 *Pacific West Coast Lecturer in Inorganic Chemistry*
1978 *Awarded the Chemistry Society Medal in Transition Metal Chemistry*
1982 *Royal Society of Chemistry Tilden Lectureship and Prize; A.R. Gordon Lecturer, Toronto University*
1983 *Karl Ziegler Gastprofessor (Max Plank Institute, Mulheim)*
J.C. Bailar Lecturer and Medal (Illinois University)
Hutchinson Lectureship (University of Rochester)
1984 *American Chemical Society Annual Award for Inorganic Chemistry*
The University Lecturer in Chemistry, University of Western Ontario
1985 *Elected Fellow of The Royal Society*

	Debye Lecturer, Cornell University
	Visiting-Professor, Wuhan University, P.R.C.
	Elected Fellow of the Royal Society
1986	*Julius Stieglitz Lecturer, University of Chicago*
	Awarded Royal Society of Chemistry Medal in Organometallic Chemistry
1987	*Frontiers of Science Lecturer, Texas A & M University*
1989	*Sir Edward Frankland Prize Lecturer*
1991	*The Glenn T. Seaborg Lecturer in Inorganic Chemistry, University of California, Berkeley*
	The South-East Lecturer in Inorganic Chemistry, U.S.A.
	The Walter Heiber Gastprofessor, University of Munich, Germany
1992	*The Karl-Ziegler Prize of the Gesellschaft Deutscher Chemiker, Germany*
1994	*Pacific Coast Lecturer, in Organic Chemistry USA, Spring, 1994*
1995	*Rayson Huang Visiting Lecturer, Hong Kong*
	Humphry Davy Medal of the Royal Societof London.
1996	*Dow Lecturer, Ottawa-Carleton Chemistry Institute, Canada*
1997	*American Chemical Society award in Organometallic Chemistry*
	Doutor Honoris Causa, University of Lisbon, Portugal
	Frank Dyer Medal, (U of New South Wales)
1998	*The Fred Basolo Medal and Lecture, Northwestern University*
	Ernest H. Swift Lectureship, California Institute of Technology
2000	*Sir Geoffrey Wilkinson Medal and Prize, (Royal Society of Chemistry)*
2001	*Lewis Lecture, Cambridge UK FMC Lecturer, Princeton*
2002- 2014	*Distinguished Visiting Professor, Hong Kong University.*
2002	*Distinguished Lecturer in Inorganic Chemistry, University of North Carolina*
	34th Camille and Henry Dreyfus Lecturer, Dartmouth College
2004	*Honorary Professor of the University of Wuhan (PRC)*
	Bert and KeggieVallee Visiting Professor, Harvard University, March 2004
2006	*Falk Plaut Lectureship, 2006. Columbia University NY*
	Honorary Doctorate Southampton University.
2007	*Prix Franco-Briitannique, Societé, Francaise de Chemie.*
2014	*Doctor of Science honoris causa 14/7/2014, University of Warwick.*
2015	*European Prize for Organometallic Chemistry 2015*
2018	*Distinguished Fellow Award, Centro de Quimica Estrutural, Lisboa, Portugal.*

Service on National Committees

Review of Synchrotron Facilities, SERC, 1992
Governing Body of the Plant Sciences Institute, AFRC, 1989-1992
Royal Society Committee C3, 1990-1994
Royal Society Committee, Exchange Scolarships (Japan, Far East) 1989-1992
RAE Chemistry Review Panel, 2002
The ERC Advanced Grant committee (Brussels) 2011, 2014.

Most recently I have been working, in collaboration with Professor Parkin, on a classification of covalently bonded compounds that has been widely accepted and is now taught at many universities. A short publication list is given below.

A New Approach to the Formal Classification of Covalent Compounds of the Elements

Malcolm.L.H. Green, Organomet. Chem. 1995, 500, 127–148.

Classification of Organotransition Metal Compounds, Gerard Parkin; Columbia University. Chapter 1, Systematic Chemistry of Covalent Compounds of the Elements.

Comprehensive Oganometallic Chemistry. Editor, R Crabtree.. 2007.

The occurrence and representation of three-centre two-electron bonds in covalent inorganic compounds.

Jennifer C. Green, Malcolm L. H. Green and Gerard Parkin,
Chem. Commun., 2012, 48, 11481–11503

4The Covalent Bond Classification Method and Its Application to Compounds that feature 3-Center 2-Electron Bonds

Malcolm L.H. Green and Gerard Parkin Struct. Bond

DOI: 10.1007/430, 2015_206.

The classification and representation of main group three-centre four-electron interactions.

Malcolm L. H. Green and Gerard Parkin,Dalton Trans., 2016, 45, 18784–1879.

Application of the Covalent Bond Classification Method for the Teaching of Inorganic Chemistry

Malcolm L. H. Green† and Gerard Parkin. Chem.Ed. . 2014, 91, 807−816.

Comment on “Hydride, gold(I) and related derivatives of the unsaturated ditungsten anion [W2Cp2(μ-PCy2)(μ-CO)2]−”

by M. A. Ruiz et al., Dalton Trans., 2014, 43, 16044
Malcolm L. H. Green

Metal–Metal Bonding in Bridging Hydride and Alkyl Compounds. Gerard Parkin.

Struct Bond (2010)136: 113–146

The Covalent Bond Classification Method has a website

www.covalentbondclass.org

This website has a library and examples of applications of the CBC method.

Abstract of recent publication.

Electrooxidation of formic acid enhanced by surfactant-free palladium nanocubes on surface modified graphene catalyst.

Kankla, P., Limtrakul, J., Green, M. L. H., Chanlek, N., Luksirikul, P.

Applied Surface Science, 471, 2019 176-184.

Direct Formic Acid Fuel Cells (DFAFCs) have been extensively focused and rapidly growing as one of alternative energy systems for portable devices and automobiles. However, power energy requires the active and selective metal nanocatalysts to perform the highest electrochemical activity. Here, we propose a nanocubic shape of palladium nanoparticles **(**PdNPs**)** decorated on functionalized graphene **(**fG**)**, where surface modification is obtained by surfactant free method**.** The 11 nm and high dispersion of Pd nanocubes **(**PdNCs**)**, which are majorly enclosed with **(**100**)** indicated by XRD and HRTEM results, are successfully deposited on functionalized graphene **(**PdNCs/fG**)** and used as an enhanced electrocatalysts for formic acid oxidation**.** Our PdNCs/fG catalyst displays a remarkable mass activity towards formic acid oxidation **(**494**.**50 A/g, over 100 times**)** compared to commercial catalysts of Pd/C, and over 20 times to PdNPs on unmodified graphene or reduced graphene oxide **(**PdNPs/rGO**).** Moreover, our catalyst exhibits better stability and higher CO resistance**.** The PdNCs/fG catalyst also generates the superior specific activity towards formic acid oxidation to 20**.**37 A/m^2**.** The study demonstrates the synergistic effect of high selective site enabled by {100} facet on PdNCs and a great potential from a support of modified graphene to Pd metal catalyst for the development of electrocatalysts in fuel cell applications.

Hydrogen, the Energy Carrier of the Future

by Eberhard Schlücker, Member EUAS

Short Biography

Prof. Dr.-Ing. Eberhard Schlücker
Chair of Institute of Process Machinery and Systems Engineering
Department of Chemical and Bioengineering
Cauerstraße 4, 91058 Erlangen / Germany

Research career

Since 4/2000 Full professor and head of the Institute of Process Machinery and Systems Engineering, University of Erlangen-Nuremberg
1997-2000 Authorized signatory, LEWA GmbH, Leonberg
1997 3-month research stay, USA
1995-1997 Head of Department R&D, LEWA, Leonberg
1989-1995 Research Assistant at the Institute for Process Technology and Machinery, University of Erlangen-Nuremberg, advisor Prof. Dr.-Ing. G. Vetter
1993 Ph.D. thesis: Optimisation of circular plastomer membranes for oscillating displacement pumps
1989 Dipl.-Ing. degree in Chemical Engineering, University Erlangen-Nuremberg
1978 - 1984 Engineer for research, design and development, deputy chief of research at company Lewa, Leonberg
1978 Ing. grad. Mechanical Engineering, Technical College Heilbronn
1974 Qualification as skilled worker in machinery

Research area / activities

Eberhard Schlücker has a wide spectrum of research interests ranging from fluid-systemdynamics and fluid acoustics to chemical and biological process technology with a main focus on pumps, compressors, high pressure and process technology. E. Schlücker holds more than 250 publications, 12 patents and is leading a group of currently 40 doctoral students.

Major activities

- *Head of research project "Bavarian Hydrogen Center"*
- *Chairman of research groups (Twin-Jet, Heart Actor, DFG Research Groups)*
- *Chairman of the research group for Ammonothermal Synthesis (DFG Proposal)*
- *Founder and coordinator of the master study program "International Project Management in Systems Engineering"*
- *Chairman of the EFCE Working Party for High Pressure Technology*
- *Member of three boards in ProcessNet (German working group for plant engineering,*
- *German working group for engineering education, German working group for high pressure processes)*
- *Member of the VDMA programme committee for the Rotating Equipment-Conference*
- *VDI Bavaria, head of section for Process Technology*
- *Member of the Advisory-Board of the Pump-User-Symposium at A+M University, Houston,Texas, USA*
- *Technical Industry consulting, several companies.*
- *Editor and reviewer for various journals (Industriepumpen und Kompressoren, Pumpen und Kompressoren, CET, etc.)*
- *Guest lecturer at various European universities*
- *In charge of ERASMUS exchange program with the university of Valladolid (Spain) and the university of Turku (Finland)*
- *Cofounder of the Agrolytix company*
- *Cofounder of the Hydrogenious company.*
- *Author of several survey reports for courts.*

Due to the observable developments of our climate (average temperature rise, glaciers and weather caprioles, to name but a few), it can no longer be denied that we humans intervene too much in the global cycles and thus cause our planet a great, perhaps even irreparable damage that future generations will have to bear. We therefore need to rethink our way of acting and should make circular economy, resource conservation and regenerative energy technology a goal for the preservation of mankind and the planet.
Energy is always a central aspect of this climate debate. The greenhouse effect, which can already be measured, is the result of this. This essay will therefore focus exclusively on the energy supply of the future, which must be based on regenerative technologies in the medium term.

1. Regenerative Energy Systems and Energy Efficiency

Renewable energy sources are only limited to sun, wind, water, biomass and geothermal energy. All five do not work everywhere, always or permanently. Therefore, we need additional storage technologies. But since the space and land we have available in the long term is not growing, but shrinking, and the population is growing at the same time, we need to launch an energy efficiency programme in addition to storage technology. There are countless possibilities for this, which we just have to want, then a lot works and profitability is certain here. But we must also be honest with each other and call ourselves the honest and real energy footprint and evaluate it on this basis. Every product has such a footprint and the goal must be to reduce or optimize it everywhere. And at the same time we have to learn to use every single bit of energy. But it should also be clear that a society that deals with this will become a highly innovative one.

2. Regenerative Energy Storage

Energy storage, on the other hand, is not so easy. Essentially, there are the following directions: Batteries, high water storage technology, the conversion of CO_2 back into fuel, the storage of hydrogen and biomass as seasonal storage. Nowadays, batteries are preferably based on lithium. However, if all energy storage systems are to be based on lithium batteries, then lithium would also become a scarce commodity in the future. High water storage cannot be built everywhere, and biomass is also necessary for our nutrition, so only biological residues should be used. This leaves the re-conversion of CO_2, for example into methanol and hydrogen, as permanently usable methods. To convert CO_2, this molecule must be cracked (393.77 KJ/mol), while the raw material for hydrogen is water, and this cleavage takes place via electrolysis (289.5 KJ/Kg).

But for methanol production hydrogen is needed anyway. So the question arises, why then take the detour to methanol, especially since CO_2 will probably have to be collected at great expense in the future and, at the same time, in times without burning fossil substances, would no longer be available simply or only from biomass sources. Therefore, a CO_2 cycle economy would have to be developed and nothing, or almost nothing, would be lost. At the same time, however, it can be seen from the energies that the hydrogen society is more energy-efficient.

Of course, geothermal energy is also a relatively sustainable source of energy, but this source of energy cannot be tapped everywhere and, in addition, the coupling with a district heating system should absolutely be realized. Otherwise the efficiencies are extremely poor. Not infrequently, less than 10% turbine efficiency is achieved here.

3. Hydrogen

Therefore, from a scientific point of view, hydrogen is the favourite for a certain basic energy supply. Hydrogen is available in water in an infinite quantity. And at the same time we do not want to consume it, but to put it into a cycle. Hydrogen is a basis for chemical processes, is very energy-rich with 33 KWh - 39.41 KWh/Kg calorific value, but also has some disadvantages for energy storage. It has the lowest density of all gases and is therefore difficult to store, but on the other hand very power dense. Therefore there is already a long tradition in dealing with hydrogen. The

first is compression to, for example, 70 MPa and storage in pressure vessels and the other is the cryogenic state (liquid hydrogen). This is the only way to achieve the necessary density for reasonable availability and storage size. Unfortunately, the high pressure or the extreme cooling requirements are not unproblematic and cost-intensive. Last but not least, there is still a certain philosophy of uncertainty attached to compressed hydrogen and also to free hydrogen.

4. LOHC – Liquid-Organic-Hydrogen-Carrier

The new method of hydrogen storage technology eliminates all these problems by storing the hydrogen in chemically bound form on a LOHC (Liquid-Organic-Hydrogen-Carrier). However, this chemical must be chemically very stable so that the thermally driven separation of the hydrogen (recovery) does not destroy the molecules. At the same time, the molecules should not produce any toxins (i.e. no nitrogen, chlorine, etc.) if they should be burnt as residues. Therefore only the pure aromatics remain. But to prevent the toxicity from becoming too great, di-benzene-toluene was chosen (Fig. 1, patented). Here 16 atoms can dock hydrogen and at the same time REACH papers (safety papers) exist for this chemical. The energy that can be stored in it is 2.1 KWh/litre, which is roughly equivalent to the amount of hydrogen in 70 MPa containers. Another advantage of this liquid is that it is non-combustible even when loaded with hydrogen. Even ignition tests with welding torches did not lead to ignition. The liquid is therefore absolutely safe.

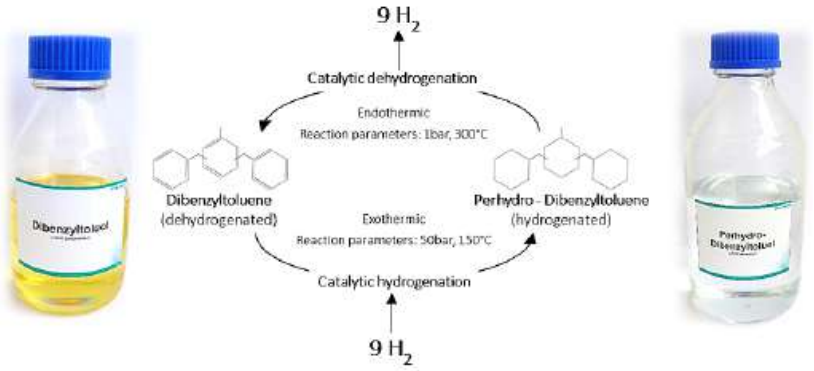


Fig. 1 Dibenzyltoluene loading and unloading process

With this storage technology, you now have a liquid that fits exactly into our heating oil and petrol infrastructure. The LOHC is oil-like and therefore pumpable. The disadvantage is certainly the relatively high temperature (300°C), which is necessary for dehydration. This was the focus of recent research and it was possible to reduce the required temperature to approx. 130°C using a clever combination of parameters (patent pending). This means that LOHC technology can now be used in many different ways, because dehydrogenation can now be carried out with the waste heat from a fuel cell, which we need to convert hydrogen into electricity. But sunlight and other waste heat sources can now also be used for this purpose.

5. The LOHC-System

The LOHC complete system from electricity to electricity consists of an electrolysis cell, a hydrogenation reactor, a storage tank, a dehydrator and a fuel cell. While the two devices electrolysis and fuel cell are technically manufactured by several companies, the optimal devices hydrogenation reactor and dehydrogenation reactor are currently still in research and development.

5.1 Hydrogenation Reactor

Figure 2 (patented) shows an arrangement of three hydrogenation reactors filled with catalyst pellets (not shown). The aim of the reactor design is to make the hydrogen gas available

everywhere in the reactor, while the LOHC is dosed as desired. Here, a structure has been developed in which the reactor tubes protrude above the ground and are open at the top for the hydrogen. The LOHC, on the other hand, is pumped in the head chamber, will enter the reactor via side boreholes according to the borehole diameter and the filling level. If a lot of LOHC is to be dosed, the LOHC level rises due to increased feed and the LOHC current increases. In addition, several boreholes can be fed as the level rises. The advantage of this design is that no additional pumps are required for the LOHC current. A further advantage is that this principle can be extended to a large number of reactor tubes in a single unit, and thus any power output can be achieved.

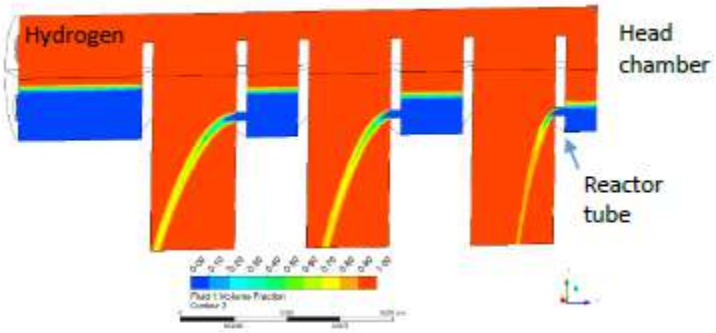


Fig. 2 Hydrogenation reactor arrangement, upper section, blue: LOHC; red: hydrogen

5.2 Dehydrogenation Reactor

The aim here is to extract the hydrogen from the LOHC and, if possible, to discharge it without pressure loss. Figure 3 (patented) shows a reactor that does this. The heating liquid is led in a spiral pipe, while the LOHC with bound hydrogen flows spirally between the pipes in a catalyst bed from the inside to the outside, and drips outside through an outlet into the sump (unload tube). Here the hydrogen has the possibility to rise above the catalyst bed in large volumes and to flow in the direction of the outlet. The pipe spirals are installed in simple vessel bottoms and can be built up as a tower on top of each other to increase the output. In addition, there is the option that this reactor form can be operated as a so-called one-reactor, which means that it can be used both as a hydrogenation reactor and as a dehydrogenation reactor.

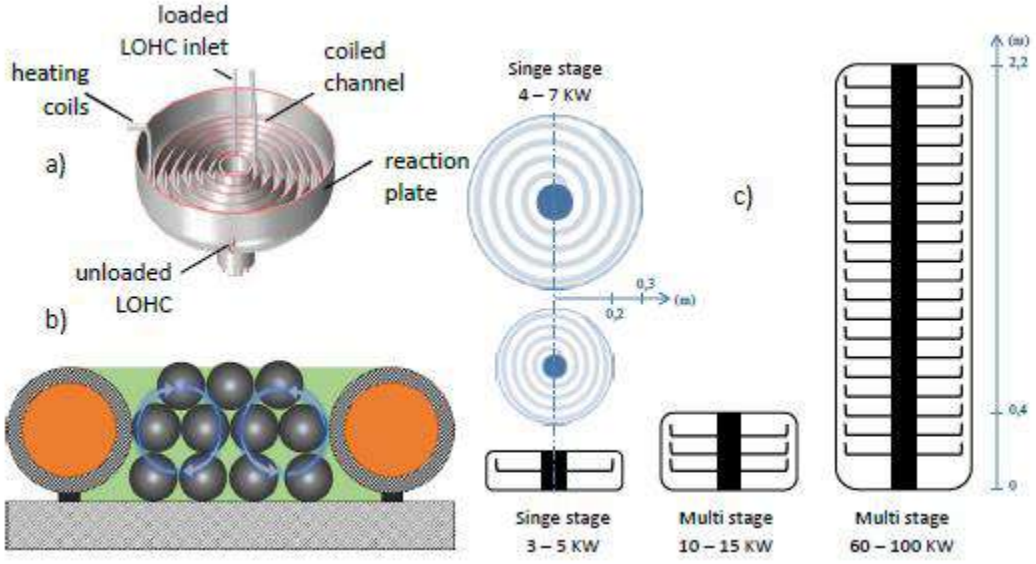


Fig. 3 Dehydrogenation reactor with spiral piping: a) Reactor element design, b) Natural convection in the catalyst bed; c) Combination of several stages for high release capacities

6. Energy Efficient possible Applications for the LOHC-Technology in the Stationary Areas

The aim, however, must be that both the oxygen (which is always produced during electrolysis) and the waste heat and hydrogen are used as far as possible.
A good example of this is sewage treatment plants. Here the oxygen can be used for the sewage process and the waste heat for the sewage sludge drying, while the hydrogen is stored and used for energy consumption (train runs with hydrogen, hydrogen filling station, etc.). It quickly becomes clear that other business models are also possible and, for example, a sewage treatment plant can become an energy seller.

The same applies to steelworks! Here, too, oxygen is needed and the waste heat could be used for preheating. But there are also possibilities in urban environments:
1) Oxygen for efficient combustion processes
2) Waste heat for local and district heating supply.
3) Waste heat utilisation for cooling devices in summer
4) Waste heat utilisation for seawater desalination
5) Waste heat for thermal production processes (extraction, rectification, reaction)65) waste heat for cooling or for greenhouses in winter (fresh vegetables in January?)
6) Upgrading the geothermal capacity with LOHC waste heat: Build the reactor into the upflow of geothermal energy. The Carnot efficiency could thus be increased from 16 - 20% to approx. 50%. And then the available residual heat could still be used for district heating. Geothermal plants could even be regulated with it.

These are just a few examples, but they already show how energy and resource networks could be created.

7. Mobile Applications

The previous exclusion criterion for mobile applications was the high dehydration temperature, which could now be reduced to 130°C (see above). This means that even cars with LOHC tanks are now conceivable (in any case already feasible for larger vehicles). Work is already underway on a train to run with LOHC [1].
Although the LOHC technology fits very well to our infrastructure, there is a small difference. Since the LOHC is not consumed, but only dehydrated, the tank has to be emptied before refuelling. But this can also mean faster refuelling cycles by simply changing the tank.

Despite this possibility, there are certainly still many mobile applications that want to use compressed hydrogen. For this reason, a compressor was developed (Fig. 4, patented) that works vertically upwards and cools the walls with bound hydrogen using the falling film of the LOHC, absorbing most of the compression heat. Thus the leakage flow through the piston seal is hardly possible because it is blocked by LOHC. The hydrogen and the excess LOHC are pumped out of the compressor and separated outside. The hydrogen gas goes to the high pressure tank (e.g. 100 MPa) while the LOHVC is led to the dehydrator, and the preheating by the compression is used for dehydration. The hydrogen thus released is returned to the compressor.

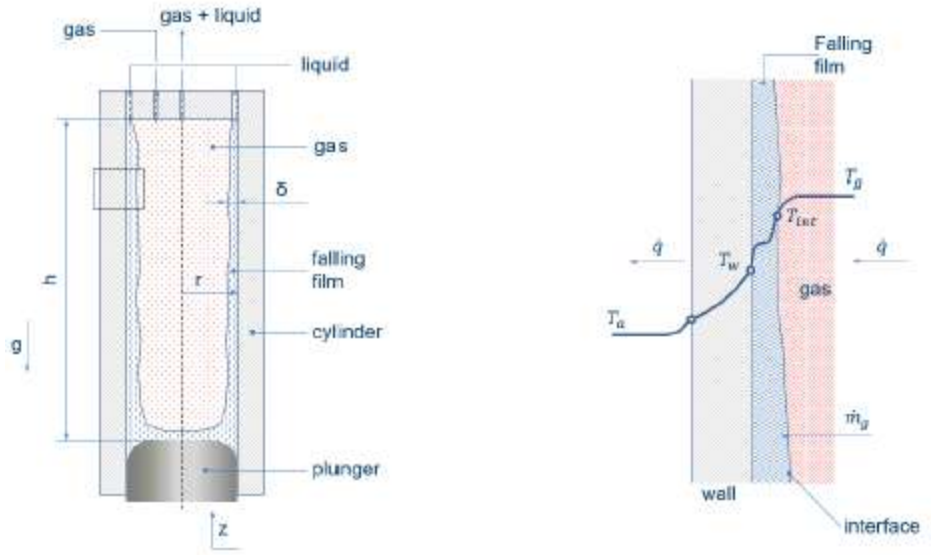


Fig. 4 Piston compressor with a barrier layer and falling film to absorb the compression heat, a) acting principle, b) heat transition calculation

8. Summary

With the new LOHC technology, a hydrogen society has come within reach. In addition, this technology solves the energy storage problem associated with renewable energy and thus contributes significantly to a sustainable energy economy.

9. Literature

[1] https://www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/DE/2018/2018-04-19-lohc-zug.html .

[2] Milella, V.O.; Koelpin, A.; Schluecker, E.: Automation of the Storing-In Part of a Hydrogen-Storage System using Liquid Organic Hydrogen Carriers (2017), https://doi.org/10.1002/ente.201700519

[3] Reuß M.; Grube T.; Robinius A.; Preuster P.: Wasserscheid, P.; Stolten. D.: Seasonal storage and alternative carriers: A flexible hydrogen supply chain model, Applied Energy, http://dx.doi.org/10.1016/j.apenergy.2017.05.050, 0306-2619/© 2016 Published by Elsevier Ltd.

[4] Brückner, N.; Obesser, K.; Bösmann, A.; Teichmann, D.; Arlt W.; Dungs, J.; Wasserscheid, P.: Evaluation of Industrially Applied Heat-Transfer Fluids as Liquid Organic Hydrogen Carrier Systems (2013), CHEMSUSCHEM, https://doi.org/10.1002/cssc.201300426

Structure and Function of the Musculoskeletal System

by David B. Burr, Member EUAS

Short Biography
David B. Burr
Distinguished Professor of Anatomy and Cell Biology, and Biomedical Engineering
Indiana University School of Medicine, and Indiana University-Purdue University Indianapolis (IUPUI)

Positions Held

2001-2002 *President, Association of Anatomy, Cell Biology and Neurobiology Chairpersons*
2007-2009 *President, American Association of Anatomists*
2008-2009 *President, Orthopaedic Research Society*
2009-2013 *Delegate, General Assembly, International Federation of Associations of Anatomists*
2013-present *Editor, Bone*
2011 *Guest Editor (with R. Graham G. Russell) for Special Issue of BONE on Bisphosphonates*
2012-2018 *Associate Vice Chancellor for Research, IUPUI*
2014-2021 *Editor-in-Chief, Current Osteoporosis Reports*
2014-2018 *Board of Directors, Federation of Associated Societies of Experimental Biology (FASEB)*
2015-2018 *Chair, Scientific Advisory Board, Fibrous Dysplasia Foundation*

Honors

1997 *Honorary Chairman, 27th International Sun Valley Hard Tissue Workshop*
2002 *First Louis V. Avioli Best Article Award, Calcified Tissue International and Springer-Verlag*
(co-recipient with Jiliang Li and Tasuku Mashiba)
2008 *Borelli Award, American Society of Biomechanics*
2009 *Fellow, American Association of Anatomists*
2010 *Chief Scientist Pro-Tempore, Hospital for Special Surgery*
2010 *Gideon A. Rodan Award for Excellence in Mentorship, American Society for Bone and Mineral Research (ASBMR)*
2013 *Named Distinguished Professor of Indiana University*
2015 *Henry Gray Scientific Award, American Association of Anatomists*
2018 *Fellow, Orthopaedic Research Society*
2018 *Albert Nelson Marquis Lifetime Achievement Award, Marquis Who's Who*

There are two broad areas of investigation that the Burr Lab has pioneered over the past 35 years. In total, these studies have led to > 70,000 citation). These areas are:

(1) The mechanical and physiological significance of skeletal microdamage to bone health
(2) The effect of current treatments for osteoporosis on bone quality, fragility and fracture risk

These areas are related, as I hope the narrative below will demonstrate, and have led to significant changes in clinical practice.

The Role of Microdamage in Bone

It is now generally accepted that microdamage in bone is a naturally occurring event, and that it is important for skeletal health. When we began to study skeletal microdamage in 1983, the existence of microdamage was not accepted as a physiological feature of bone. Although Harold Frost had first proposed its existence in 1960, "cracks in bone" were considered to be an artifact of preparation. We were the first to demonstrate conclusively that microcracks in bone are not artifactual, but are a common physiologic occurrence consequent to normal human activity and bone loading. We were able to validate the *en bloc* basic fuchsin technique for staining microcracks in vivo. This technique remains the gold standard for assessing microdamage in bone. Once we had proven the technique for exposing them, the phenomenon of microdamage was observed in multiple labs using different techniques, and their occurrence in now accepted by nearly everyone, including U.S. government regulatory agencies such as the FDA (see below). Following our demonstration of this in 1990, the primary orthopaedic research society in the U.S. – the ORS – went from having no scientific sessions on the subject of microdamage in bone, to having as many as five sessions devoted to this topic in a single year.

Once the existence of microdamage was proven as a real event, most investigators tended to think of it as only a mechanical event. However, we were able to show in two papers as early as 1985 that microdamage is "targeted" for repair by the bone remodeling system. These papers showed that microcracks were signaling for their own repair. We now know that the role of microdamage in bone mechanics is less important to skeletal health than its physiological role. We also know that this occurs through the following process: microdamage disrupts canalicular communication among osteocytes, which are the sensor cells in bone. This causes apoptosis of osteocytes close to the damage; if apoptosis is prevented, repair of the damage does not occur. Osteocytes in areas of damage then upregulate the production of RANKL, which is a cytokine related to osteoclast differentiation and activation. Thus, osteocytes in areas of microdamage recruit osteoclasts to specific areas to remove damage; because the osteoclasts are coupled to osteoblasts, new bone is formed once the old bone is removed, and the damaged region is repaired. This process is fundamental to maintain bone's strength and prevent fracture.

Treatments for Osteoporosis

It follows from the work with microdamage repair that suppressing the normal repair of microdamage using anti-resorptive agents to prevent bone loss might be detrimental to bone health. In 1995, alendronate (Fosamax) was the first approved bisphosphonate (BP) used for the treatment of osteoporosis. The BPs can prevent fracture especially in postmenopausal women with low bone mass by preventing further bone loss and deterioration of architecture. My lab has been engaged for the past 20 years in studies to examine the effect of suppressed bone remodeling on the qualities of the bone itself. Although BPs are effective at preventing bone loss and do reduce the risk of fracture in most people, it seemed to us that the inhibition of damage repair could represent a significant risk factor for women on long-term BP therapies. Using a pre-clinical animal model, we demonstrated in a series of papers beginning in 2000 that treatment with BPs

could reduce the amount of energy required for bone to fracture (ie reduce the mechanical "toughness" of bone. We have published numerous papers on this topic, and now other labs have found similar results. The results have been clear: we find that suppressing bone turnover with BP treatments increases bone mineral density (BMD) and makes the whole bone stronger, but at the expense of the properties of the tissue matrix, which becomes more brittle and can absorb less energy per unit of mass before it breaks. Thus, although bone strength may be increased, fracture risk can be increased too.

In 2006, orthopaedic surgeons and others began to detect an increased incidence of femoral shaft fractures, especially in women taking BPs for long periods of time. Femoral shaft fractures are not that common (this is the largest bone in the body), and these had "atypical" characteristics different from other femoral fractures. This was consistent with our observations that BP treatment makes bone more brittle and reduced the energy required for bone fracture. I was asked to Co-Chair an International Task Force for the American Society for Bone and Mineral Research (ASBMR) to define atypical femoral fractures and provide recommendations for BP treatments. The initial Task Force report was key to the FDA decision in 2011 to require pharmaceutical companies to place warnings on BP labels that these agents, when taken over a long time, could be associated with symptoms that can result in atypical femoral fractures.

Because atypical femoral fractures are now considered to be a type of stress fracture (rather than an "osteoporotic" fracture), we investigated the effect of BP administration on the cyclic fatigue life of bone. This work shows that treatment with BPs, at least at high doses, is associated with a 3-fold reduction in fatigue life, and demonstrates the proof-of-principle that BPs could be implicated in the pathogenesis of atypical femoral fractures.

This work has altered clinical practice related to the administration of BPs and other anti-resorptive agents to patients. Whereas in the past, these were used to prevent bone loss in younger women in their 50's, most physicians now will not prescribe them until there is significant loss of bone, ie bone mass that is greater than 2.5 standard deviations less than normal healthy pre-menopausal women. Further, most physicians recommend considering a drug holiday following 5 years of treatment.

Because severe suppression of osteoclastic bone resorption is associated with these negative consequences, we now have begun to explore the idea that it is possible to improve bone material properties and reduce fracture risk without interfering with normal cellular activity, ie without significantly preventing bone remodeling. This approach would prevent the deleterious effects that severe suppression of remodeling has on bone properties, with its increased risk for atypical femoral fractures. This work could lead to the development of a new class of drugs to treat bone fragility.

Certain Selective Estrogen Receptor Modulators (SERM) such as raloxifene reduce fracture risk nearly as much as the BPs, but without severe suppression of bone remodeling (20% with SERMs vs. 70-90% with BPs) or large increases of BMD (2% vs. 12% over three years). The fracture efficacy of the SERMS is far greater than what would be predicted based solely on its effect on bone mineral density (BMD). In a series of preclinical studies, we documented that raloxifene improves material-level toughness of bone despite little/no change in BMD. More recent work has demonstrated that this

mechanical property enhancing effect of raloxifene is cell- and estrogen receptor-independent. We incubated bone beams without living cells for 2-14 days, and consistently found significantly improved bone material properties, predominantly increased toughness, the exact property that BPs affect negatively and that leads to atypical femoral fractures. This work and subsequent work showed that raloxifene increases bound water within the matrix and alters strain transfer between the organic (collagen) and mineral (hydroxyapatite, HAP) portions of the matrix.

We then determined that raloxifene directly interacts with the bone tissue, something never shown before. Because a mechanism independent of the bone cells and the estrogen receptor (ER) pathway activation could represent a unique pharmacological approach to reducing osteoporotic fractures, we wished to identify the structural features within the benzothiophene nucleus of raloxifene that are responsible for this compound's direct interactions with bone tissue. We applied a comprehensive approach using multiple complementary biophysical techniques including Nuclear Magnetic Resonance (NMR), Mass Spectrometry (MS) and Fourier transform infrared spectroscopy (FTIR) in order to shed light on the interaction of SERMs with bone and its components, and the structural requirements that mediate the material-level biomechanical properties and hydration of bone. Through the use of these multiple and complementary biophysical techniques, we showed that raloxifene interacts specifically with the organic component or the organic/mineral composite, and not with hydroxyapatite. Structure–activity studies revealed that the basic side chain of raloxifene is an instrumental determinant in the interaction with bone matrix through electrostatic interactions and through hydrophobic interactions (van der Waals) with the collagen molecule. Furthermore, in silico prediction of the potential binding sites on the surface of collagen revealed the presence of a groove with sufficient space to accommodate raloxifene analogs, meaning that other drugs with similar structure could be identified as potentially effective cell-independent agents to reduce fracture risk.

These studies show for the first time that the relationship between hydration and bone mechanics holds true when hydration is increased, and most importantly, that hydration can be affected positively through pharmaceutical treatment. It further demonstrates that raloxifene positively affects tissue-level biomechanical properties of bone through non-cell mediated effects on hydration. These results could open avenues to engineering of new compounds that do not act through cellular processes, but specifically target the mineral and collagen interface to increase hydration and energy absorption and reduce fracture risk of bone, without negative side effects.

We also were involved in many pre-clinical (animal model) studies leading eventually to the approval of teriparatide (rhPTH1-34), the first FDA approved anabolic agent for the treatment of osteoporosis in humans. All other pharmaceutical agents used to treat osteoporosis prevent bone loss by suppressing bone remodeling, and its first phase, bone resorption. However, teriparatide is the only agent to date that treats osteoporosis by causing net bone formation. It does this in two ways. Upon initial treatment, there is an anabolic window in which bone formation is stimulated, but bone resorption is not; ie, resorption and formation are uncoupled, allowing formation to occur without prior

resorption. Following this phase (4-6 months), resorption is increased, but bone formation is increased more, "overfilling" the cavities that have been resorbed and creating a net bone formation at each remodeling site. The anabolic effect of teriparatide was shown in a series of papers using rats, rabbits, and monkeys. The rabbit studies were particularly influential in demonstrating that the later increase in bone resorption occurred primarily near the marrow cavity, and therefore did not have a transient negative effect on the mechanical strength of the bone.

Bone Fatigue and Stress Fractures

Because of my interest in the mechanical adaptation of bone, we began to study the origin and pathogenesis of stress fractures. One notable early set of experiments involved applying strain gages to my tibia to measure bone strains that occurred during vigorous activities. I was only the second person in the world to have strain gages applied in vivo to my bone. These data led to a number of other studies with Israeli collaborators to evaluate the role of impact and muscle fatigue on bone strain. We developed a rabbit model of stress fracture by adapting the rabbit impact loading device that was used to study osteoarthrosis to create tibial stress fractures in rabbits. This work has become particularly pertinent recently with the observation that atypical femoral fractures are a type of insufficiency stress fracture. This observation, in combination with our other work showing that long-term bisphosphonate (BP) use could cause deterioration in the mechanical and material properties of bone, led to more recent investigations on the effect of BP administration on the fatigue life of bone. This work shows that treatment with BPs, at least at high doses, is associated with a 3-fold reduction in fatigue life, and demonstrates the proof-of-principle that BPs could be implicated in the pathogenesis of atypical femoral fractures.

Is Alzheimer a Runaway Autoimmune Disease? And How to Cure It?

by Alain L. Fymat, Member EUAS

Short Biography

DR. ALAIN L. FYMAT is a medical-physical scientist and an educator. He is the current President/CEO and Institute Professor at the International Institute of Medicine & Science with a previous appointment as Executive Vice President/Chief Operating Officer and Professor at the Weil Institute of Critical Care Medicine, California, U.S.A. He was formerly Professor of Radiology, Radiological Sciences, Radiation Oncology, Critical Care Medicine and Physics at several U.S. and European Universities. Earlier, he was Deputy Director (Western Region) of the U.S. Department of Veterans Affairs (Office of Research Oversight). At the Loma Linda Veterans Affairs Medical Center, he was Scientific Director of Radiology, Director of the Magnetic Resonance Imaging Center and, for a time, Acting Chair of Radiology. Previously, he was Director of the Division of Biomedical and Biobehavioral Research at the University of California at Los Angeles/Drew University of Medicine and Science. He was also Scientific Advisor to the U.S. National Academy of Sciences, National Research Council, for its postdoctoral programs tenable at the California Institute of Technology, Jet Propulsion Laboratory. He is Health Advisor to the American Heart & Stroke Association, Coachella Valley Division, California. He is a frequent Keynote Speaker and Organizing Committee member at several international scientific/medical conferences. He has lectured extensively in the U.S.A, Canada, Europe, Asia and Africa. He has published ~ 435 scholarly scientific publications and books. He is also Editor-in-Chief, Honorable Editor or Editor of 71 medical/scientific Journals to which he regularly contributes. Dr. Fymat is a Board member of several institutions, a member of the New York Academy of Sciences and a reviewer for the prestigious UNESCO Newton Prize, United Kingdom National Commission for UNESCO.

With interest in Africa, Dr. Fymat is also associated with the Society for the Advancement of Science in Africa (SASA) where he holds several executive positions (Board Vice Chair; Executive Council Member; Scientific Directorate Director; Scientific Committee Chair). He was also Chair of its Conference Programs (2013 in Polokwane, South Africa; 2014 in Kampala, Uganda; 2015 in Toronto, Canada; 2016 in Nairobi, Kenya; and 2017 in Kigali, Rwanda).

RESEARCH INTERESTS

DR. FYMAT's current research interests are focused on neurodegenerative diseases (Alzheimer, Parkinson, epilepsy, dementias and others), oncology (glioblastoma), molecular/precision/personalized medicine, and nanomedicine & nanobiotechnology. These are represented in his latest book From the Heart to the Brain: My Collected Works in Medical Science Research (2016-2018), pp 592, Tellwell Talent Publishers, 2018. The following contribution is a provocative suggestion as to the root cause of Alzheimer ,and possibly other neurodegenerative diseases, together with suggested curative approaches.

Is Alzheimer a Runaway Autoimmune Disease? And How to Cure It?

There are approximately 400 known neurological diseases, some of which classified as mental disorders. A number of these disorders are mediated by a disruption or failure of the blood brain barrier. Unfortunately, the convergence between the barrier studies and clinical investigations has historically been limited. Nonetheless, in the case of Alzheimer, I posit that the compromised integrity of the barrier is a component of the etiology of the disease, not a consequence of it. I further submit that the root cause of the disease is the brain's autoimmune system having gone rogue (a sort of "run away" effect) in its unsuccessful attempts to maintain brain homeostasis between the antagonistic synaptoblastic and synaptoclastic pressures. The cure would be to balance these pressures by regulating the system rather than fiercely combating either the hyper-excited synaptoblastic pressures or/and suppressing the synaptoclastic ones.

Over the past few decades, Alzheimer disease, once considered a rare disorder, has emerged from obscurity to become a major public health problem. Based on a lack of treatment, it has been generally considered as an irreversible, progressive brain disease that slowly destroys memory and thinking skills, eventually even the ability to carry out the simplest tasks. It is a chronic neurodegenerative disorder of poorly (or not) understood cause(s). Based on identified risk factors, several theories (hypotheses) have been propounded for its cause(s) beyond genetics (early onset familial disease, late onset sporadic disease): cholinergic, amyloid, viral or fungal infection, tau, neurovascular, neuroinflammation, neurodevelopmental, cardiovascular, gum disease infection, dysfunction of oligodendrocytes, and others related to lifestyle, diet, and the environment, and many others. Such a wide array of hypotheses is by itself indicative of our lack of true understanding and knowledge of the disease notwithstanding the fact that the disease has been identified since 1901 and has been the subject of a considerable number of publications dealing with it (in excess of 50,000, according to some authors).

Despite claims by some research clinicians, there are currently no known treatments if only to stop or reverse the progression of the disease. Some of these alleged "treatments", including the advocated program ("DESS": Diet, Exercise, Stress, Sleep, and variations on this theme) are palliative in nature, temporarily improving symptoms,... while the disease progresses unabated. One must keep in mind that *risk is not causation and risk management is not treatment, only palliation*! Research has rather focused on diagnosing the condition before symptoms begin. Thus, a number of biochemical tests have been developed to attempt earlier detection including analysis of the cerebrospinal fluid for beta-amyloid (Aβ) or tau proteins and preventive anti-body vaccination. Neuroprotective agents (e.g., Al-108, PBT2 and TNFα receptor-blocking fusion protein etarnacept) have also been designed. Further, among the more than 400 pharmaceutical treatments having been investigated or in advanced clinical trials, putative pharmaceutical therapies attempt to treat the underlying disease pathology such as by reduction of Aβ levels (e.g., by apomorphine, investigational immunotherapy, or vaccination) and inhibiting tau aggregation (e.g., with methylthionium chloride and dimebon). Again, however helpful, such treatments are not curative. Still other "softer" methodologies involve meditation and anti-fungal infection of the brain.

Putative immunological therapies, based on the concept of training the immune system to recognize, attack, and reverse the deposition of Aβ have been designed. Unfortunately,

such a surrogate end-point has not been clinically demonstrated to cure the disease, i.e., even after the amyloid plaques had been removed, the disease symptoms persisted and the disease itself continued its deleterious progress. Additionally, immunotherapeutic agents have been found to cause some concerning adverse drug reactions. Still further, one important limitation of active and passive immunotherapy as currently practiced is the low amount of antibodies that can pass the blood brain barrier (this may, however, be overcome by coupling antibodies to the peptide penetratin). In distinction with the antibodies employed, several small molecules have been designed to readily pass the barrier while delivering therapeutic compounds at the right locations in the right dosage amounts, heralding a new treatment approach. This is also what nanomedicine and nanotechnology promise to do. However, while the technology is now well known, its application to neurodegenerative disorders has not yet been undertaken.

In brief, while palliative treatments are available, neurodegenerative disorders in general, and Alzheimer in particular, have generally been declared as incurable. The reason is that we have not yet been able to identify the etiology and deep biology of their root cause(s). This situation is reminiscent of that for other diseases, particularly cancer. It was not until after we came to the realization that cancerous cells like healthy cells from which they evolve are braided in our genome, and that cancer is not an organ disease but the result of multiple genetic mutations, i.e., understanding the deep biology of cancer, that we have made great strides in cancer treatment and cure. Witness the emergence of Immuno-Oncology and the recent U.S. FDA-approved use of chimeric antigen receptor (CAR) T-cells. Immunotherapy has been successful in inducing long-term remissions of hard-to-treat cancers. The early identified protein receptor on the surface of T-cells (cytotoxic T-lymphocyte antigen 4, CTL-4) and a molecule (programmed death 1, PD-1) led to astonishing tumor shrinkage and increased survival, particularly in metastatic melanoma. Thus, anti CTL-4 and anti PD-1 have opened up new vistas in tumor treatment. Beyond that, genetically modified patient's T-cells and PD-1 molecules promise to be even more effective in specifically tailoring the treatment to the patient along the precepts of personalized medicine.

To employ immunotherapy in the case of Alzheimer implies that the brain has immune capabilities. In the past, owing to the presence of the brain's protective barriers at the interface between the central nervous system and the periphery, and their muted response to neuroinflammation, it had been widely assumed heretofore that the brain (and, more generally, the central nervous system) is immune-privileged. However, in contrast to this earlier dogma, it is now evident that these immune capabilities do exist. The brain's vaguely understood component of the immune system is normally able to handle, treat, and overcome any adverse pathologies developing therein. It fails when the insult is so unsurmountable as to cause the immune system to go haywire. Despite the protective mechanisms of the barriers, the capacity for immune-surveillance of the brain is maintained, and there is evidence of inflammatory signaling at the brain barriers that may be an important part of the body's response to damage or infection. This signaling system appears to change both with normal aging and during disease. Changes may affect organic phenomena (or diapedesis) of immune cells and active molecular transfer, or cause rearrangement of the tight junctions and an increase in passive permeability across barrier interfaces. In parallel with immunotherapy as an emergent therapy of cancer, I advanced earlier the opinion that brain immunotherapy should also become a similar therapy for

brain cancers and neurological disorders, providing a paradigm shift in our therapeutic approach to brain cancer and these disorders.

I now posit that the root cause of Alzheimer is the brain's very autoimmune system that had run amok in its attempts to maintain brain homeostasis. This balancing process consists of two phases: (a) the synapse- building or "synaptoblastic" phase: neurons sport receptors called amyloid precursor proteins that grab hold of netrin-1 (molecules floating by in the intercellular environment) and send signals to the neurons to keep them healthy and functional; and when this process fails (b) the synapse-destroying or "synaptoclastic" phase: it defaults to opposite signals that instruct the neurons to commit suicide and to the amyloid precursor proteins to produce more Aβ thereby outnumbering netrin-1. As a consequence, the amyloid precursor proteins are less likely to grab netrin-1 and more likely to keep grabbing Aβ. Any effective treatment for Alzheimer should therefore include a method to rebalance the synapse building and dismantling phases, not enhancing or destroying either phase.

The approach advocated here would be to regulate the underlying autoimmune system (not to either enhance it immeasurably or suppress it totally), to boost in a measured manner the synaptoblastic signals while at the same time taming down the synaptoclastic signals. This idea builds upon work done in diabetes type I, an incurable disease so far, in which the autoimmune system is taught to tolerate the insulin-producing cells of the pancreas so that it does not destroy the diabetic patient's ability to produce the glucose-regulating insulin. The similar idea forms the basis of various clinical trials for treating other incurable diseases such as multiple sclerosis and Graves disease. The overarching purpose is to tame down the hyperactive autoimmune system by employing molecules that can induce an immune response (antigens) or engineered immune cells that can train the autoimmune system to tolerate the process or tissue it is on track to damage. This idea has the potential to cure a range of autoimmune disorders, including especially neurological and neurodegenerative disorders and particularly Alzheimer. As stated earlier in the case of cancer and brain tumors, this requires a deep understanding of the molecular basis of autoimmunity, including brain and central nervous system immunity, as well as advances in genetic engineering and cell-based therapy. Caution must nonetheless be exercised as deploying the immune system to treat certain diseases can also potentially trigger other autoimmune diseases, e.g., in the case of cancer, it may additionally trigger rheumatoid arthritis and colitis.

The main immune players are the regulatory T-cells (T_{reg}), which act as the brakes of the immune system. Similarly to other T-cells, T_{reg}-cells rein in the immune cells that are doing damage. It has been suggested that the body can be made to produce the T_{reg}-cells required to dampen a certain autoimmune response by dosing people who are affected with the same antigen or antigens that the immune system wrongly interprets as a reason to attack. This was tested for multiple sclerosis, demonstrating less brain inflammation. The approach is similar to vaccination without the immune-system stimulants called adjuvants that are usually included in vaccine formulations. Here, antigens can induce a calming effect through T_{reg}-cells.

There may be other ways to temper a rogue autoimmune system. For example, in cell-based therapy, a patient's T_{reg}-cells can be removed from the body, engineered to respond to specific antigens that have been wrongly recognized by the immune system as being

foreign, and then returned. This is the very principle of the FDA-approved chimeric antigen receptor (CAR) T-cells (here T_{reg}-cells) that have been applied to cancer treatment. They can also be used to dampen harmful inflammation.

In conclusion, a number of known neurological and neurodegenerative disorders are mediated by a disruption or failure of the blood brain barrier. While understanding the nature of the barrier's role (and also the role of multi-drug resistance) is imperative in designing treatments, the fundamental question of whether the compromised integrity of the barrier is a component of the etiology of the disease under consideration or a consequence of it remains unanswered. I have advocated for the former instance. Like in other diseases (diabetes, cancer, etc.), we have been hampered by our imperfect understanding of the underlying biology and, in desperation, have too soon declared such diseases as “incurable”. However, the realization that the brain and the central nervous system are endowed with their own immune system, accompanied by the greater understanding of the mechanism of autoimmunity, and the advent of cell-based therapy will empower us to conceive other treatment strategies and even cures as I have attempted to do here in the case of Alzheimer. The main immune players, the regulatory T-cells (T_{reg}), which act as the brakes of the immune system, can be so manipulated (engineered) as to temper and regulate the autoimmune system and train it to tolerate (rather than fiercely combat) the opposing pressures to achieve brain homeostasis. There may also be additional ways to temper a rogue autoimmune system such as, for example, emulating cancer immunotherapy with CAR-T cells but with CAR-T_{reg} cells for the neurodegenerative diseases of interest.

Rough Sets (RS) and Interactive Granular Computing (IGrC)

by Andrzej Skowron, Member EUAS

Short Biography

Andrzej Skowron, *an EurAI (ECCAI) and IRSS Fellow, and the Member of EU Academy of Sciences, received the Ph. D. and D. Sci. (habilitation) from the University of Warsaw in Poland. In 1991 he received the Scientific Title of Professor. He is a Full Professor in the Systems Research Institute, Polish Academy of Sciences as well as in the Digital Research Center of Cardinal Stefan Wyszyński University in Warsaw. He is Emeritus Professor in Faculty of Mathematics, Computer Science and Mechanics at the University of Warsaw. Andrzej Skowron is the (co)author of more than 400 scientific publications and editor of many books and volumes of conference proceedings. His areas of expertise include reasoning with incomplete information, approximate reasoning, soft computing methods and applications, rough sets, rough mereology, granular computing, intelligent systems, knowledge discovery and data mining, decision support systems, adaptive and autonomous systems, perception based computing, and interactive computational systems. He was the supervisor of more than 20 PhD Theses. In the period 1995-2009 he was the Editor-in-Chief of Fundamenta Informaticae, an international journal. He is in the Editorial Boards of many others international journals. Andrzej Skowron was the President of the International Rough Set Society from 1996 to 2000. He has delivered numerous invited talks at international conferences including a plenary talk at the 16th IFIP World Computer Congress (Beijing, 2000), a keynote talk at the 8th Joint Conference on Information Sciences (JCIS 2005) (encompassing 12 individual conferences and workshops) (USA, 2005), an invited talk at the 2006 IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT 2006) and on Web Intelligence (WI 2006) (Hong Kong, 2006), and a plenary talk at the 2nd World Congress on Biologically Inspired Computing (Japan, 2010). He was serving as (co-)program chair or PC member of more than 200 international conferences. He was involved in numerous research and commercial projects including dialog-based search engine (Nutech), fraud detection for Bank of America (Nutech), logistic project for General Motors (Nutech), algorithmic trading (Adgam), control of UAV (Linköping University), and medical decision support (e.g., in Polish-American Pediatric Clinic in Cracow). Andrzej Skowron was in the ICI Thomson Reuters/ Clarivate Analytics lists of the most cited researchers in Computer Science (globally) in 2012, 2016, 2017.*

In the article are outlined two areas of research in which Andrzej Skowron is active for many years. These are: Rough Sets (RS) and Interactive Granular Computing (IGrC). In both of these areas he has been recognized by the research community as one of the leading researchers with numerous results related to developing foundations and methods to be used in real-life applications.

1. **Rough Sets** (see, e.g., http://rsds.univ.rzeszow.pl/home and https://www.roughsets.org/)

The rough set approach was proposed by Professor Zdzisław Pawlak in 1982 as a tool for dealing with imperfect knowledge, in particular with vague concepts. The philosophy of rough set is founded on the assumption that with every object of the universe of discourse some information (data, knowledge) is associated. Objects characterized by the same information are indiscernible (similar) in view of the available information about them. The indiscernibility relation generated in this way is the mathematical basis of rough set theory. This understanding of indiscernibility is related to the idea of Gottfried Wilhelm

Leibniz, according to whom objects are indiscernible if and only if all available functionals take on them identical values. However, in the rough set approach indiscernibility is defined relative to a given set of functionals (attributes).

Any set of all indiscernible (similar) objects is called an elementary set, and forms a basic granule (atom) of knowledge about the universe. An arbitrary union of some elementary sets is referred to as *crisp* (precise) set. If a set is not crisp then it is called *rough* (imprecise, vague). It is to be noted, that due to the computational complexity of searching for relevant crisp sets for the problem of vague concept approximation, the searching is usually restricted to a feasible subfamily of the family of all possible unions of elementary sets. Each rough set has *borderline cases*, i.e., objects which cannot be classified with certainty as members of either the set or its complement. Obviously, crisp sets have no borderline elements at all.

The rough set theory has gained interest of many researchers and practitioners from all over the world. The rough set approach is of fundamental importance in artificial intelligence and cognitive sciences, especially in machine learning, data mining and knowledge discovery, pattern recognition, decision support systems, expert systems, intelligent systems, multiagent systems, (complex) adaptive systems, autonomous systems, cognitive systems, conflict analysis, risk management systems, etc. Many methods based on rough sets have wide applications in many real life projects. Rough sets have established relationships with many other approaches such as fuzzy set theory, granular computing, evidence theory, formal concept analysis, (approximate) Boolean reasoning, multicriteria decision analysis, statistical methods, decision theory, matroids. Despite of the overlap with many other theories, the rough set theory may be considered as an independent discipline on its own right. There are reports on many hybrid methods obtained by combining rough sets with other approaches such as soft computing (fuzzy sets, neural networks, genetic algorithms), statistics, natural computing, mereology, principal component analysis, singular value decomposition or support vector machines. The main advantage of the rough set theory in data analysis is that it does not need any preliminary or additional information about data like probability distributions are needed in statistics, basic probability assignments are needed in evidence theory, and a grade of membership or the value of possibility is needed in fuzzy set theory.

The results of Andrzej Skowron related to rough sets concern, e.g., logical aspects of rough sets, methods of approximation of complex vague concepts, searching for relevant approximation spaces, sorites paradox, relationships of rough sets with other approaches (e.g., fuzzy sets, Dempster-Shafer theory, information flow, reaction systems, (approximate) Boolean reasoning), developing of efficient heuristics based on Boolean reasoning for data reduction (using different kinds of reducts), discretization, symbolic value grouping, hierarchical learning, discovery of concurrent models from data, etc.

2. **Interactive Granular Computing (IGrC) (see, e.g., publications of Andrzej Skowron on https://dblp.uni-trier.de/pers/hd/s/Skowron:Andrzej related to IGrC)**

Rough sets play a crucial role in the development of Granular Computing (GrC). The extension of GrC to Interactive Granular Computing (IGrC), developed by Skowron with co-workers, requires generalization of the basic concepts such as *granules* to *complex granules* (including both physical and abstract parts), information (decision) systems to

interactive information (decision) systems as well as methods of inducing hierarchical structures of information (decision) systems to methods of inducing hierarchical structures of interactive information (decision) systems. IGrC not only takes into account the granularity of information as used by humans in problem solving, but also includes interactions with the real physical world. Computations in this model are realized on interactive complex granules and that *must* be based on consequences of the interactions occurring in the physical world. With the interaction rules learned from the acquired data, computations can approximate concepts related to the expectations of complex granules (e.g., agents). IGrC can be treated as the basis for developing: (i) Wisdom Technology, in particular for approximate reasoning (called *adaptive judgment*) about properties of interactive computations, (ii) context inducing and discovery of structured objects, (iii) reasoning about changes, (iv) process mining (this research was inspired by Professor Pawlak in 1992), (v) perception based computing, (vi) risk management in computational systems, etc.

Andrzej Skowron's work is in line with Fredrik Brooks' proposition (Brooks was a recipient of the Turing Award, the most prestigious award in Computer Science). According to him:

"Mathematics and the physical sciences made great strides for three centuries by constructing simplified models of complex phenomena, deriving, properties from the models, and verifying those properties experimentally. This worked because the complexities ignored in the models were not the essential properties of the phenomena. It does not work when the complexities are the essence."

Consequently, computational models related to complex phenomena cannot be constructed solely in an abstract mathematical space — they must also take into account continuous interactions with the real physical space. In particular, computational models cannot ignore the laws of physics, as is well known from, e.g., quantum computing. The models have to be created adaptively through a process of continuous interaction with reality. The objects in the abstract space must be able to adapt according to the perceived changes in the external physical reality.

The main aim of the current research by Skowron and co-workers is to develop the IGrC models over objects called complex granules. More compound granules are represented by networks of interacting less compound granules changing with time. Any IGrC model must also be able to direct the attention of complex granules (e.g., agents) to focus on significant fragments of reality that are measured by sensors, or that are subject to performing the actions and plans. Results of interactions are collected in information systems (e.g., decision tables), which constitute some fragments of the complex granules. Following another Turing Award winner, Leslie Valiant, these tables are then aggregated to create new complex granules as computational building blocks for cognition.

There are many challenges related to IGrC. Some of them are related to *adaptive judgment.* One of the main aim of *adaptive judgment* performed by complex granules (e.g., agents) is to derive conclusions for selection of action(s) which should be currently initiated (or terminated). The actions are activated on the basis of satisfiability of some complex vague concepts labelled by actions. It should be noted that these concepts are drifting with time. Adaptive learning of such concepts based on judgment is a great

challenge. The whole process towards inducing approximation of these vague concepts labelled by actions, which are initiated on the basis of satisfiability of these concepts, may be treated as a process of discovery of a *complex game*. In such a game the concepts (together with assigned relevant judgment mechanisms to them) can be treated as players who by using their judgment mechanisms are deriving arguments *for* and *against* the satisfiability of these concepts on the basis of information about the perceived situation. Next, there are other judgment mechanisms, in the hands of a judge, that can be used to resolve conflicts among the collected arguments to select the winning player (concept). Then action labelling the winning concept is initiated.

It should be also noted that the complex vague concept approximation should be based on judgment rather than on partial inclusion of sets only. The former approach is much more general than the latter one. The approach based on judgment is especially relevant when in data analysis it is required to have a deeper judgment about the perceived complex situation related to classification of complex vague concepts. The approach based on partial containment of sets is not satisfactory for dealing with many real-life applications, where more advanced judgment should be made to identify the perceived situation and classify it relative to the complex vague concepts. Hence, there is the need for further developing new logical tools for reasoning based on judgment toward approximation of complex vague concepts and to rough sets based on adaptive judgment performed over computations on complex granules. This, in particular, creates a room for extensions of rough sets to adaptive rough sets and rough sets over distributed networks of granules changing with time.

It is worthwhile mentioning that the proposed model is in agreement with the recently raised discussions about the Turing test for intelligence. In addition to linguistic aspects and reasoning, it incorporates perception and actions, and it follows what Leslie Valiant's calls *ecorithms*.

The proposed model of computation based on complex granules seems to be of fundamental importance to developing of intelligent systems dealing with complex phenomena, in particular in such areas as Data Science, Internet of Things, Wisdom Web of Things, Cyber Physical Systems, Complex Adaptive Systems, Natural Computing or applications based on Blockchain Technology, etc.

Developments in Civil Engineering Infrastructure Materials

by Serji Amirkhanian, Member EUAS

Short Biography

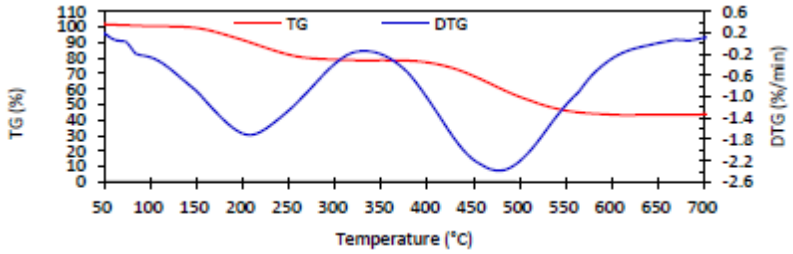
Serji Amirkhanian was the Mays Professor of Transportation and the Director of the Asphalt Rubber Technology Services (ARTS) in the Department of Civil Engineering at Clemson University until June of 2010, before he started his international consulting activities. At this point, he is the CEO and President of Asphalt Technologies LLC and was the Director of Research and Development for Phoenix Industries of Las Vegas. He is a Professor of Civil Engineering at the University of Alabama, Tuscaloosa in addition to be a Research Faculty at Tongji University (Shanghai) and a Professor of Civil Engineering at Wuhan University of Technology (Wuhan, China). He is also an Adjunct Research Faculty at UNLV, an Adjunct Professor at Arizona State University (ASU), an Adjunct Faculty at IIT Madras (India), and a Researcher of materials at NTNU, Norway. He is the Co-Director of the International Recycled Rubber Products Initiative at UNLV. In addition, he is the recipient of the 100 Foreign Expert award from Hubei Province, China. He has conducted research for over 30 years in construction materials area, specially hot mix asphalt area, for many private companies, SC DOT and Federal government. He has obtained over $25 million in funding for his research activities and teaching the DOT certification courses. He has published over 325 papers refereed journal papers, conference papers and research reports. He has also published several book chapters and has served as the co-editor of two books. He has conducted over 300 presentations around the US and the world presenting his research findings. He has supported and has advised over 170 students and over fifteen post-doctoral scholars. He is a member of many national and international engineering associations. He regularly reviews journal papers for many journal publications around the world in addition to serving on many thesis documentations from students from other countries. He has conducted 11 international conferences in the use of recycling materials in many applications around the world (US, EU and China). He has been involved with many recycling field projects, in civil engineering area, all over the world including China, Vietnam, Canada and many states in the United States. He has conducted consulting and/or research work for the United Nations (UNIDO), the World Bank, Honeywell International, BMW, Michelin, Owens Corning, among many others.

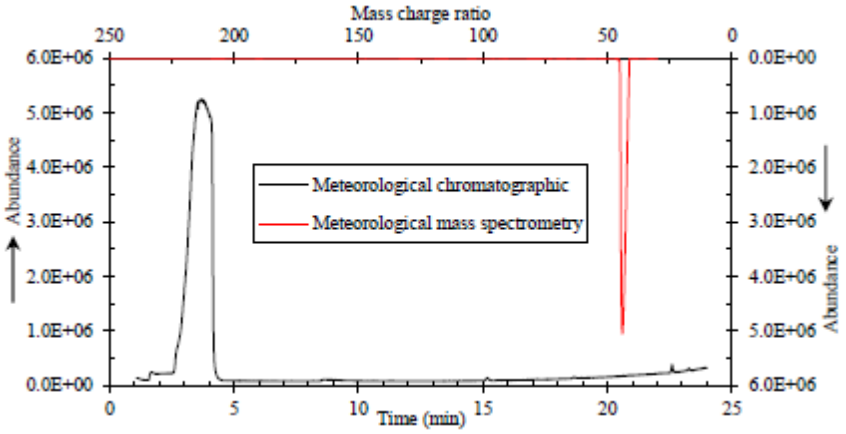
Professor Amirkhanian's research work has been divided into several areas including: a) polymer applications in infrastructure applications; b) recycling of construction materials; and c) new developments in polymer materials in Civil Engineering. There are many polymers being used or evaluated in asphalt industry. Some of his research topics and findings are described below.

Graphene oxide (GO), is a precursor for grapheme, which has atomic thickness and two-dimensional sizes in the tens of micrometer range or larger and its molecular structure is roughly the same as the grapheme. In addition, it has the excellent gas and liquid

blocking performance and reported certain conductivity. Currently, GO, for its excellent structure and functional properties, is widely used in many industries such as carbon-based electronics, impermeable membrane, gas sensors, and polymeric composite materials. For instance, some researchers have demonstrated that GO layered structures could maximize the gas-diffusion path length; therefore, significantly decreasing the gas flux through layered composite films. Other researchers reported a significant improvement in the modulus and tensile strength of the butadiene-styrene-vinyl pyridine rubber by utilization of GO. While, others have determined that GO has an extremely large specific surface area, high modulus, in conjunction with water solubility and versatile surface chemistry. Therefore, they have concluded that it could be used as the reinforcing additives for various polymers. For this research work, two types of asphalt binders (base asphalt of 80/100 penetration grade and SBS modified asphalt) and two levels of GO contents (1% and 3% by weight of asphalt binder) were utilized in preparing the GO modified asphalt (GO MA) by melt blending method. Initially, the following testing were conducted to study the interaction between GO with asphalt: a) Fourier transform infrared spectroscopy analysis (FTIR), b) X-Ray diffraction analysis (XRD) and c) gas chromatography-mass spectrometer (GC-MS). Then, the thermo gravimetric (TG) analysis was performed to determine the thermal properties of GO and its effect on the of asphalt binders.

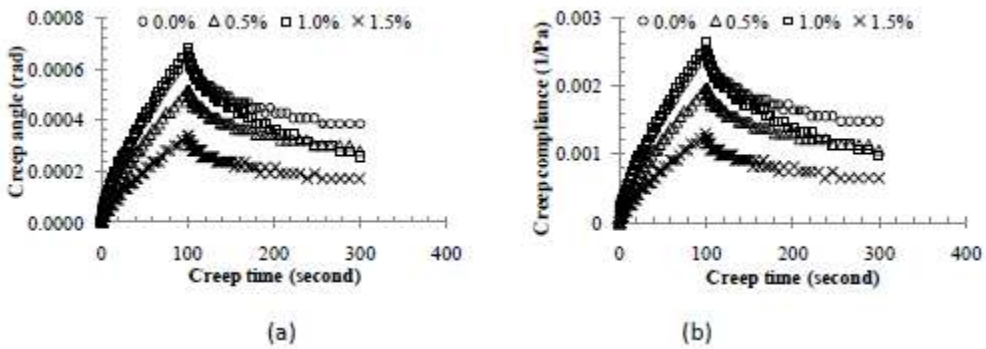
Before the GC-MS analysis of GO MA, in order to ensure the starting decomposition temperature of GO, the thermal properties of GO were studied by thermal analyzer in the temperature range of 50 °C to 700 °C (figure below). The results indicated that the mass loss of GO, with the increase of temperature, GO mainly has two mass loss stages. The temperature range of stage 1 is 154 °C to 334 °C, and total quality decrease in the stage 1 is 21.52%, the maximum mass loss rate at 208 °C. The temperature range of stage 2 is 334 °C to 629 °C, and total quality decrease in the stage 2 is 35.15%, the maximum mass loss rate at 478 °C. In general, the heating temperature of asphalt during production and mixing processes is lower than 200 °C, so the temperature range of the stage 1 combustion process is the key to influence and explain the GO-asphalt interaction. The GC-MS test was used in identifying the gases released during the preparation of GO MA. For instance, the GC-MS image of the 90A+3%GO is shown in figure below. There is an obvious peak at the mass charge ratio of 44 in the gas mass spectrometer image demonstrating the gas released during preparation process is the carbon dioxide (CO_2). Combining with thermal analysis result of GO, it can be demonstrated that the CO_2 is generated form the decomposition of the oxygen-containing functional groups in GO. The gas chromatography shows that the CO_2 is released mainly at the time range of 2.5 min to 4.5 min, and there is almost no gas after 4.5 min, which shows that, when given a fixed content of GO, the amount of CO_2 is limited due to the limited oxygen-containing functional groups.





The conclusions indicated that a) the gas that was released during preparation process was CO_2. There was no chemical reaction between the GO and asphalt binders, the CO_2 was produced by the decomposition of the GO. After being mixed with asphalt binders, the lamella structure of the GO was completely stripped and scattered to a single layer in 90A and SBS MA; b) the separation test demonstrated that GO/90A and GO/SBS MA have good storage stability; c) the GO can improve the anti-rutting performance of 90A and SBS MA in the temperature range of 30 °C to 80 °C; d) BBR analysis demonstrated that the GO could improve the low temperature anti-cracking performance of asphalt binders; e) the GO could improve the fatigue cracking resistance performance of 90A and SBS MA; and f) the GO could improve the thermo-oxidative aging resistance performance of the modified binders.

In another study, the effects of a short-term and long-term aging procedures on the rheological properties of an asphalt binder containing various percentages of carbon nano particles were investigated. The results of creep compliance for two grades of binders are shown below. In general, the results indicated that creep and creep recovery results illustrate that the nano particles can effectively improve the deformation resistance of the tested asphalt binders due to the reduction of compliance value at pressure aging vessel (PAV) aged states. In addition, the test results illustrated that the creep angle and compliance values of the binders with or without nano particles have obviously recoveries after PAV aging process since it exhibits an obvious decrease after removing a 100-second loading.



Typical creep compliance, (a) PG 64-22; (b) PG 52-28

In another study, the feasibility of using a multilayer feedforward artificial neural network (ANN) to predict the fatigue life of the modified asphalt mixtures was studies. Fatigue, associated with repetitive traffic loading, is considered to be one of the most significant distress modes in flexible pavements. The fatigue life of an asphalt pavement is related to the various aspects of hot-mix asphalt (HMA). When an asphalt mixture is subjected to a cyclic load or stress, the material response in tension and compression consists of three major strain components: elastic, viscoelastic, and plastic. The tensile plastic (permanent) strain or deformation, in general, is responsible for the fatigue damage and consequently results in fatigue failure of the pavement. A perfectly elastic material will never fail in fatigue regardless of the number of load applications. The fatigue behavior of a specific mixture can be characterized by the slope and relative level of the stress or strain versus the number of load repetitions to failure. The strain- and energy-dependent fatigue prediction models of the mixtures are shown below, left and right land table; respectively.

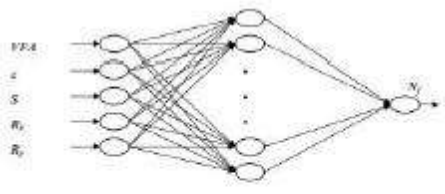
Ambient	Traditional predicting model	R^2	COV (%)
VFA (5 °C)	$N_f=1.0E(-13)*\varepsilon_0^{3.6}*e^{20.2*VFA}*S_0^{2.2}$	0.37	66
A.V. (5 °C)	$N_f=4.8E(-2)*\varepsilon_0^{-0.2}*e^{-0.1*V_0}*S_0^{0.7}$	0.09	28
VFA (20 °C)	$N_f=3.3E(5)*\varepsilon_0^{6.5}*e^{20.9*VFA}*S_0^{1.9}$	0.36	82
A.V. (20 °C)	$N_f=1.9E(26)*\varepsilon_0^{5.8}*e^{-0.4*V_0}*S_0^{0.2}$	0.53	106
Cryogenic			
VFA (5 °C)	$N_f=1.3E(5)*\varepsilon_0^{8.7}*e^{-0.1*VFA}*S_0^{2.9}$	0.13	47
A.V. (5 °C)	$N_f=3.6E(11)*\varepsilon_0^{7.2}*e^{-0.2*V_0}*S_0^{2.3}$	0.32	78
VFA (20 °C)	$N_f=1.7E(34)*\varepsilon_0^{9.1}*e^{-0.5*VFA}*S_0^{4.02}$	0.27	51
A.V. (20 °C)	$N_f=3.9E(20)*\varepsilon_0^{3.4}*e^{-0.2*V_0}*S_0^{0.6}$	0.36	61

Note: N_f=fatigue life; ε_0=initial flexural strain; VFA=volume of voids filled with asphalt binder; V_0=initial air-void content in percentage; S_0 =initial mix stiffness; and A.V.=air voids.

Ambient	Traditional predicting model	R^2	COV (%)
VFA (5 °C)	$N_f=0.74*e^{13.8*VFA}*\varepsilon_0^{0.01}$	0.22	57
A.V. (5 °C)	$N_f=4.9E(4)*e^{-0.1*V_0}*\varepsilon_0^{0.2}$	0.09	37
VFA (20 °C)	$N_f=4.1E(-4)*e^{21.8*VFA}*\varepsilon_0^{2.6}$	0.49	135
A.V. (20 °C)	$N_f=1.1E(5)*e^{-0.3*V_0}*\varepsilon_0^{1.9}$	0.42	121
Cryogenic			
VFA (5 °C)	$N_f=1.1E(4)*e^{-0.2*VFA}*\varepsilon_0^{0.5}$	0.04	31
A.V. (5 °C)	$N_f=2.4E(4)*e^{0.2*V_0}*\varepsilon_0^{0.4}$	0.21	78
VFA (20 °C)	$N_f=4.0E(4)*e^{-0.2*VFA}*\varepsilon_0^{0.9}$	0.40	84
A.V. (20 °C)	$N_f=8.1E(4)*e^{-2.5*V_0}*\varepsilon_0^{1.0}$	0.27	66

Note: N_f=fatigue life; ε_0=initial flexural strain; VFA=volume of voids filled with asphalt binder; V_0=initial air-void content in percentage; S_0 =initial mix stiffness; and A.V.=air voids.

Experimental data on the fatigue life of rubberized asphalt concrete mixtures containing reclaimed asphalt pavement obtained in this study were used for model development. The results showed that the traditional regression-based models were unable to predict the fatigue life of modified mixtures accurately. The ANN approach, as a new fatigue modeling method used in this study, has been shown to be effective in creating a feasible predictive model. The established ANN-based models were able to predict the fatigue life accurately, as evidenced by high R^2 values regardless of the type of crumb rubbers and test conditions. The results indicated that ANN-based models are more effective than the regression models. The ANN models can easily be implemented in a spreadsheet, thus, making it easy to apply. Both strain-dependent and dissipated energy-dependent methods were effective in predicting the fatigue life of the modified mixtures when additional input variables are included in the ANN-based models. The following three-layer feedforward neural network architecture was used to develop the prediction models.



R_b = the percentage of rubber in the binder; R_p = the percentage of RAP in the mixture; ε = initial flexural strain; VFA = Volume of Voids filled with asphalt binder; S = initial mix stiffness; N_f = fatigue life.

Innovative Investigations of PrandtlPlane

by Aldo Frediani, Member EUAS

Short Biography

Prof. Aldo Frediani, graduated in Aerospace Engineering at Pisa University (Italy) in 1972; in 1985 became full professor at the Aerospace Engineering School of the University of Rome "La Sapienza" at the Aero-Missiles Structures chair, where he succeeded to prof. Luigi Broglio, director of the School and father of the "San Marco project" (the first European space program with vehicles in orbit). In 1990 he was called by the University of Pisa to occupy the Aeroelasticity chair at the Aerospace Engineering Department.

The teaching activities concerned different fields of the Aerospace Engineering, such as theoretical mechanics, aerospace structures, aircraft design, machine design, Aerodynamics, Aeroelasticity; he gave lectures at foreign universities and at courses organized by the European Community. The research activities are evidenced by the publication of about 200 publications regarding different fields of Engineering both theoretical and experimental, as: fatigue of aeronautical metallic structures, theoretical aspects of linear and non linear Facture Mechanics, wind tunnel tests on aerodynamics of aircraft and of industrial components, theoretical aerodynamics of multi-wings configurations. Prof. Frediani designed and carried out static and fatigue tests on bogies of trains and different railways elements, including the Italian high speed trains. He is the owner many national and international patents, in railways systems, aircraft innovative concepts, machines for the Italian museum of Mathematics in Florence.

The activities related to the new transport aircraft configurations have led to the acquisition of international patents on innovative aircraft configurations in the USA and Europe. With regards to these matters, prof. Frediani has been the coordinator of a project financed by the Ministry of University of Italy, of European projects for the development of a hybrid propulsion, of a general aviation aircraft and, starting from May 2017, he is the scientific coordinator of a Horizon 2020 European Project for the development of a medium sized civil transport aircraft. This concept could modify the air transport of the future, owing to the high aerodynamic efficiency, to the great increment of payload of aircraft with limited wing span, the reduced fuel consumption and noise, the possibility of introducing new fuels. In the field of photovoltaic cells for electric propulsion, he has defined configurations admissible for flying at altitudes exceeding 20Km for the territory observation and telecommunications purposes; a general mathematical model has been formulated for this aircraft.

Prof. Frediani had a long collaboration with the School of Mathematics and, starting from the beginning of 90s he organized several international workshops at the School of Mathematics at the Ettore Majorana Centre in Erice dedicated to the Applied Mathematics and to the Aerospace Engineering with the general scope of integrating these two fields. He was awarded of the Cherubino Prize by the University of Pisa and during the period 1993-2002, he holded the charge of Pro-Rector of the same University. He also contributed to the creation of the Italian Museum of Mathematics in Florence; he designed, realized and patented a mechanical system based on the Generator of Equations by D'Alambert for this Museum. He collaborated also with the Italian Institute of Nuclear Physics of Physics on the design of the CMS system at CERN Institute.

The progress of civil aircraft has produced one of a most significant business worldwide and a means of social progress of mankind. This success is the result of the scientific and technological advancements in terms of basic disciplines in mechanics, performances and safety of flight; afterwards, the advancements in aerospace has been spread among all the other engineering disciplines.

The performances of modern aircraft allow to cross a continent in some hours of flight or to reach a new continent in about half of a day. A modern civil transport aircraft can fly continuously for a 25-30 years of operating life, with a small probability of failure (one catastrophic accident in a couple of million flight or a failure of a primary component in one million years or so). The civil air transport has changed the mutual knowledge of people as never occurred in the history of mankind. Not more than some decades ago, many people experienced a tragedy for the immigrations of their loved ones, being aware to see them for the last time in their life; but not today, thanks to the efficiency air transport. Many people will have the possibility to travel and to access to global commerce; the air traffic allows a global mean of understanding other persons, to reduce the risks of conflicts, to enhance mutual links, to enjoy new holidays, to enhance the standard of life etc.

The air traffic in terms of seat-km or tone-km, is increasing from many decades and it is foreseen to increase more than 5% per year in the future, especially along the so-called point to point (short-middle ranges), where the air traffic is estimated to double in less than two decades.

But, together with the air traffic, also the noxious emissions grow faster and faster; the combustion of one kilogram of kerosene produces, among other emissions, about 3.2 kg of Carbon Dioxide (CO2) which accumulates in the atmosphere and contributes to produce the global warming effect. The attention towards the problems of climate has grown significantly in the last year and many financial resources have been devoted for improving the green sky. In Europe, ACARE (Advisory Council for Aviation Research and Innovation in Europe) has defined the requirements to be fulfilled by the aviation of the future in order to cut air pollution and noise and enhance the safety of aircraft.

These recent ACARE requirements on a greener and safer transport aviation will never be fulfilled by conventional airplanes, which have grown up to their maximum potential and have very small margins to improve their efficiency. One possible solution to be explored is the introduction of new “disruptive” aerodynamic configurations with the ambition to be a first milestone towards the introduction of unconventional civil aircraft capable to meet the challenging requirement and to become a standard for the future air transport.

Several new aircraft concepts were investigated in EU projects, mainly related to the Blended Wing Body, Truss Braced Wing and PrandtlPlane concepts. The first and the second concepts are based on the reduction of the induced drag (the drag connected with the generation of lift) by improving the wing span; these concepts cannot be suitably applied when a reduction of the wing span is required. The major increment of air traffic of the future is foreseen in the case of the short-medium ranges (known also as “point to point” air traffic, typical of the low cost companies), in airports of ICAO category C, where the maximum wing span is restricted to 36m; at the same time, the increment of this traffic will saturate the airports and, thus, we need to increase the payload capacity of the aircraft. The two constraints of major efficiency and larger capacity cannot be fulfilled by aircraft based on the two concepts cited before.

The third concept is PrandtlPlane, in honour of Ludwig Prandtl, the father of Aerodynamics. In 1924 Prandtl introduced the concept of Best Wing System (BWS), the

lifting system with the minimum induced drag among all possible wing systems. BWS is a box wing in the front view made of two horizontal wings and two vertical wings, properly designed, connecting the tips together. Due to the Munk theorems in Aerodynamics, the best wing system concept is valid in the case of swept wings so that the concept can be applied also to the case of transonic speed, the most commercially convenient for the civil air traffic.

A PrandtlPlane has positive lift on both wings and can be stable in any flight condition, the stall speed is lower than any equivalent monoplane, the cabin services and the emergency evacuation is the same of the well experienced conventional aircraft, the stall phenomenon is very smooth (and the safety enhanced), pitch control is innovative and efficient, freight capability is higher than in today airplanes, many solutions are possible for engines, different propulsion systems can be adopted more easily, as liquid hydrogen or hybrid solutions.

Many research activities are conducted on the PrandtlPlane concept, where Aerodynamics, Flight Mechanics, Propulsion, Structures etc, are finalised to introduce new ideas and tools for design and MultiDisciplinary Optimization (MDO).

With reference to the class of the point to point air traffic, the PrandtlPlane concept allows to improve the passengers of more than 50% compared to the present aircraft of reference, without improving the overall dimensions of them, to reduce the turnaround time in the airports, to reduce the vorticity on the runways (and allowing to increment the number of flights and the safety during take- off). The PrandtlPlane concept can be applied to design any dimension aircraft, from small to extra large ones. Aircraft with a payload of 1400 passengers can be designed, meanwhile the overall dimensions can be contained into a square of 80x80m, typical of present airports. New fuels could be adopted for the propulsion of PrandtlPlane in the future as, for example, liquid Hydrogen or liquid Methane.

In 2017, the European Commission has financed a project (Parsifal) in the framework of a Horizon 2020 call on “disruptive configurations”; in this context, the project aims at defining an innovative optimum aircraft, where optimum is a new concept where the needs of airline and airport companies and aircraft manufacturers and society are taken into account. Versatility, high performances, increased safety, reduction of costs and environmental impact are the expected characteristics, achievable in the medium term. OVERALL OBJECTIVES of the PARSIFAL Project is the implementation of the necessary scientific, technological and engineering background to design an innovative aircraft configuration, for the civil aviation of the future.

Compared to traditional aircraft, PrandtlPlane has the same aerodynamic efficiency with a lower wingspan, and can improve the payload capability beyond today limits, while being fully compatible with present airports. This is advantageous not only for the very large aircraft that challenge the 80x80m box constraint, but also for smaller size ones. Most of the present claims are not based just on paper studies, but stems also from experimental work carried out by the proposers, including tests on a small aircraft based on the PrandtlPlane configuration, as it will be explained more ahead. It is in fact “surprising” that the simple and “old Prandtl concept” has been left lying for many decades: some works have been done in the past on the matter, but they are far too low to let this important concept exploitable from the industrial point of view: it is time to pass from a "potential" to a "concrete" PrP aircraft in Europe. For this reason, some years ago the proposers started a research activity on this subject, as it will be explained more ahead. Results are very promising, but it is still needed a qualitative jump in research to be able to aspire to give a decisive turn to the knowledge and above all to the necessary means to

enable the Prandtl concept to become the pillar of the "Standard European Aircraft" of the next future.

Versatility, high performances, increased safety, reduction of costs and environmental impact are the expected characteristics, achievable in the medium term. OVERALL OBJECTIVES of the PARSIFAL Project is the implementation of the necessary scientific, technological and engineering background to design an innovative aircraft configuration, named "PrandtlPlane" (PrP), for the civil aviation of the future. This configuration is based on the implementation of a box-wing system, where front and rear wings are connected at their tips to form a closed wing, also known as "box-wing". This aerodynamic configuration, when properly designed, has the minimum induced drag among all the systems with the same span and total lift, which significantly improves the overall aerodynamic efficiency. The principles and the benefits of this configuration will be detailed later in this document. Due to its particular wing layout and the associated aerodynamics (and also structural) benefits, the PrandtlPlane configuration has the potential of achieving the aforementioned targets on performance, safety and environment, by means of the following advantages: larger payload than conventional aircraft can be lifted, without any increase of the wing span (with positive consequence on airport operations); lowest induced drag, with consequent reductions in required thrust, fuel consumption, noxious emissions and noise, especially at take-off; lower structural weight, in particular of the fuselage, because of the double support of the wings; scalability to aircraft of different size. Contrarily to other unconventional configurations of interest, such as Blended Wing Body, the PrP configuration can be applied to aircraft of any size, from 2 seaters to ultra large airliners; suitability to distributed propulsion architectures supported by the availability of double set of wings for engine installation; Increased safety due the inherently superior stall performance of the box wing system and the possibility to provide pitch control using a pure moment (with no change in lift). In addition, the new aircraft configuration will be the most convenient, in a very long time perspective, to face new challenges as, for example, extra large fuselages like very big cargo, capable of transporting intermodal containers; it will be easily scalable to different dimensions for the transport of passengers from short to long distances; it will be suited for distributed propulsion systems along the full wings span (e.g. the possibility of implementing a distributed electric architecture which takes energy from a heat source); alternative and/or combined power sources, like liquid hydrogen, will be also a possibility for PrP. Such a highly performing configuration will lead to unique, cheap and efficient solutions for air transportation out of the reach of conventional configurations, for different aircraft categories such as ultra large airplanes (even bigger than A380) or twin aisle regional aircraft. Such aircraft will be a key point to extend the industrial leadership of Europe. Moreover, in view of the complexity and novelties of the matters involved, new fields of research in aeronautical sciences (aerodynamics, flight mechanics, aeroelasticity, structures, engines, new fuels, etc.) will be investigated. SPECIFIC OBJECTIVES of the PARSIFAL Project are stated here below. Clear and measurable, they will be scrupulously monitored during the Project: definition of the PrandtlPlane configuration: both structure and distributed propulsion system will be investigated, giving a final statement of the most promising configuration (aircraft geometry, structural solutions, aeroelastic verifications, etc) in the case of a 250 passengers "baseline configuration". Scaling procedures of the basic aircraft: the PrandtlPlane will be conceived in such a way that the basic configuration can be up/downscaled and adapted with minor modifications to develop "family individuals".

The Dawn of a New Era of Topobiology Initiated for Life Science and Biomedicine

by Yiguo Zhang, Member EUAS

Short Biography

2010.07-present : Full Professor of Cell Biochemistry and Topogenetics, in the College of Bioengineering & Faculty of Sciences, Chongqing University, China;
2008.01-2012.10 : Senior Fellow (Co-PI) of Cancer Biology and Chemoprevention, in the Medical Research Institute, Ninewells Hospital & Medical School, University of Dundee, Scotland, UK;
2006.10-2010.06: Adjunct Professor of Life Science, at the School of Life Sciences, Zhengzhou University, Henan, China;
2007.12, PhD awarded by University of Dundee, Scotland, UK; And elected as a Fellow of the Royal Society of Medicine (FRSMed);
2003.05-2007.12: Senior Scientific Officer of Cancer Chemoprevention, in the Biomedical Research Institute, Ninewells Hospital & Medical School, University of Dundee, Scotland, UK;
1999.07-2003.04: Research Fellow of Molecular and Cellular Biology, in the Hormel Institute, University of Minnesota, USA.
1995.07-1999.06: Lecturer of Pathophysiology, in the School of Basic Medicinal Sciences, Henan Medical University, China (having merged into Zhengzhou University in 2000);
1992.09-1995.06: Postgraduate for a Master Degree of Medicine awarded by Henan Medical University in 1995;
1984.08-1992.08: Resident Physician and Qualified Doctor-In-Charge, working in the Hospital affiliated to the Fourth Bureau of the Ministry of Railways, China;
1981.09-1984.07: Medical Student, in Xinyang School of Clinic Medicine, Henan, China.

Original Discovery of Topobiology

At first, topobiology was conceived by Gerald M. Edelman (awarded for Nobel Prize in Physiology or Medicine in 1972), for study of the place-dependent (morpho)regulation of cells resulting from interactions of molecules at cell surfaces with those of other cells and/or substrate during the development and growth, leading to distinct cell differentiations of species-specific tissue patterns and animal forms[(1)]. Later, by conceptual integration of this framework with molecular cell biology, genetics and/or epigenetics, the term '***topobiology***' is hence extended from the morphogenesis to membrane-protein topogenesis and other information flow problems to gene regulation in biology insomuch as to dictate the identification of cell types, as well as integrity of differential tissues and organs (thereby, also called ***topogenetics***). Such a new concept of topobiology is initiated by Yiguo Zhang and his colleagues[(2-11)]; this has been appreciatively recognized by Mikhail Bogdanov together with William Dowhan[(12)], Gökhan S. Hotamisligil[(13)], Elke Krüger[(14)] and Carolyn R. Bertozzi[(15)].

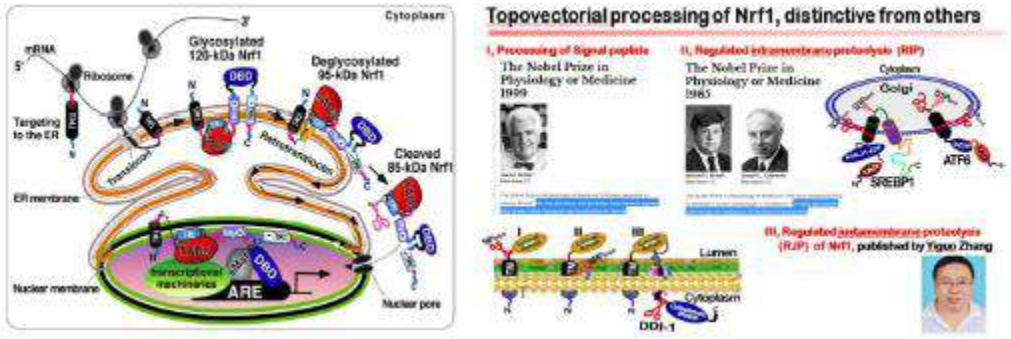


Figure 1. *Left schematic* presentation of topovectorial processing of membrane-bound Nrf1 transcription factor controlling cell homeostasis and organ integrity, as well as epithelial-mesenchymal transition (EMT) [8,16]. Such topologically-regulated juxtamembrane proteolysis (i.e. Model III, in *right panel*)[10] is completely distinctive from the processing of signal peptides (i.e. *Model I*) and regulated intramembrane proteolysis of both ATF6 and SREBP1 (i.e. *Model II*).

In the original work of Yiguo Zhang focusing on Nrf1 topobiology (Figure 1), its topology-decisive elements (called ***topogons***) were identified[2-7] to determine the positioning and repositioning of its functional domains in distinct subcellular compartments. Of note, its transactivation domains (TADs) is, while required for biological cues, dynamically retrotranslocated from the lumen of endoplasmic reticulum (ER) across membranes into extra-ER cyto/nucleoplasmic sides before regulating target genes. Such temporospatial changes in ***topovectorial*** processing of Nrf1 enable it to commit for its successive post-translational modification and proteolysis in order to give rise to distinct ***topoforms*** and/or multiple ***proteoforms*** with different or even opposing activities. The topologically-***regulated juxtamembrane proteolysis*** of Nrf1[10] (i.e. *Model III*, right panel of Figure 1) is significantly different from the processing of signal peptides[17] (*Model I*, found by Günter Blobel for the 1999 Nobel Prize in Physiology or Medicine) and the regulated intramembrane proteolysis of ATF6 and SREBP1[18] (i.e. *Model II*, *this was done* by collaboration of Joseph L. Goldstein and Michael S. Brown, in addition to their early discoveries concerning the regulation of cholesterol metabolism awarded for the 1985 Nobel Prize in Physiology or Medicine).

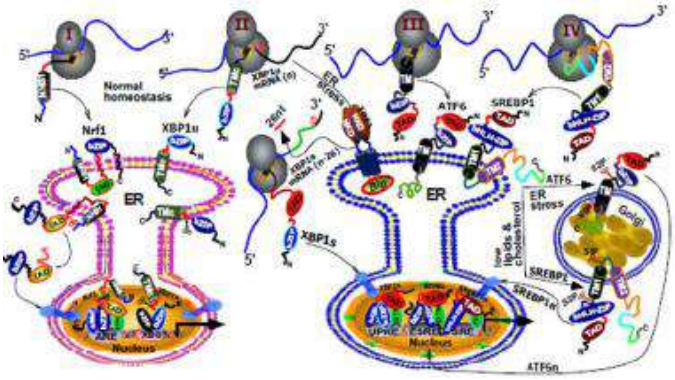


Figure 2. Four types of membrane-bound transcription factors Nrf1, XBP1u, ATF6 and SREBP1, with distinct topologies within and around the endoplasmic reticulum, before being dislocated into the nucleus[19].

It is of significant importance to note that Nrf1 is a dynamic moving membrane-protein entailed with distinct topologies, which are dictated by *topogons* integrated in distinctive orientations within and around the endoplasmic reticulum before being dislocated into the cytoplasm and nucleus[2-11]. Such dynamic ***topovectorial*** regulation of Nrf1, abiding by the ***positive-inside rule***[20] and/or charge balance rule[12], confers it to be clearly distinguishable from those of ATF6, SREBP1, and XBP1u (Fig. 2). The highly homologous protein of Nrf1 (called ***Nach***) is identified as a novel subgroup at an **early evolutionary stage** of the CNC-bZIP family factors from the marine bacteria to human beings[21]. In addition, an variant mutant of Nrf1 (called ***Nrf1D***) is determined as the ***first candidate secretory transcription factor*** in the blood plasma, alongside with its precursor identified to exist as a unique redox-sensitive transmembrane CNC-bZIP protein in hemopoietic and somatic tissues[19].

Collectively, distinct temporospatial phase transitions of Nrf1 with certain topoforms moving in and out of ER membranes comply with the ***principle of topological conservation***. This topovectorial regulation of Nrf1 dictates its post-translational modification, proteolytic processing and overall transcriptional activity[4-7,10,11]. Notably, Nrf1 is an ER membrane sensor that is central to cholesterol homeostasis[4,6,10,13], besides redox homeostasis and proteostasis[8,9]. Taken altogether, the work on the topobiology of Nrf1 from signal sensor to target gene expression is promising to open a new era of life science and biomedicine, and also create a new path for topological, rather than quantitative and qualitative, analysis.

By contrast with the water-soluble Nrf2 factor that is accepted as a master antioxidant regulator against cellular stress, Nrf1 is indispensable for embryonic development and healthy growth during life process. This fact demonstrates that Nrf1 paves a solid basis for construction of cell homeostasis and plasticity, as well as a robust integrity of differential tissues and organs at certain steady-states maintained during adaptation to various stresses [8,9] (Figure 3, *left panel*). Recently, Yiguo Zhang's group unraveled a panoramic view of opposing and unifying inter-regulatory cross-talks between Nrf1α and Nrf2 at different layers of the endogenous regulatory networks from multiple signaling towards differential expression profiling of target genes[25]. Collectively, Nrf1α acts a dominant tumour-repressor by confining Nrf2 oncogenicity. In turn, Nrf2, though as a tumor promoter, can also directly activate the transcriptional expression of Nrf1 to form a negative feedback loop (Figure 3, *right upper panel*).

Furthermore, the cytoprotective activity of Nrf2, as a two-edged sword involved in both cancer prevention and progression, is critically controlled by Keap1, which is an adaptor subunit of Cullin 3-based E3 ubiquitin ligase and also is a key sensor for oxidative and electrophilic stresses (Figure 3, *left panel*). More interestingly, Dr. Zhang's group has reported a novel naturally-occurring mutant of Keap1 (called Keap1$^{\Delta C}$)[26], lacking most of its C-terminal Nrf2-interacting domain essential for inhibition of the CNC-bZIP factor. Thus, Keap1$^{\Delta C}$ retains no or less ability to inhibit Nrf2, so that it functions as a dominant-negative competitor of Keap1 against its inhibition of Nrf2 due to its antagonist effect on Keap1-mediated turnover of Nrf2 protein (Figure 3, *right lower panel*).

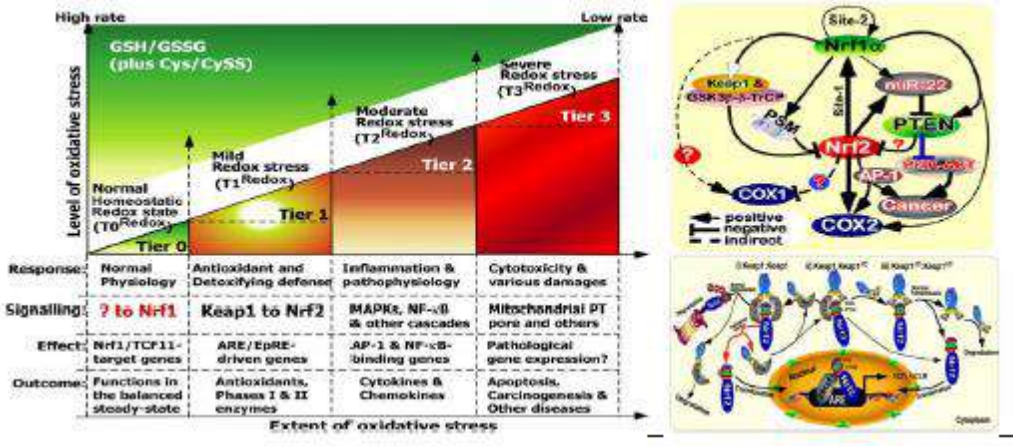


Figure 3. ***Left schematic diagram*** of distinct contributions of Nrf1, Nrf2 and Keap1 to cytoprotection against the hierarchical oxidative stress[9]. In addition, an inter-regulatory model between Nrf1 and Nrf2 is proposed to explain mutual opposing and unifying cross-talks at distinct levels[25] (*right upper panel*). Another model is also proposed to give a better explanation of Keap1$^{\Delta C}$, acting as a dominant-negative competitor of Keap1 against its inhibition of Nrf2[26] (*right lower panel*).

In addition, it should also be noted that, in the beginning of the identification of structural and functional domains in Nrf1 and its signature motifs, Dr. Zhang ***firstly discovered that this protein is anchored within the ER membranes through its NHB1 peptide folded in a correct orientation of N_{cyto}/C_{lum}*** (i.e. the N-terminal and C-terminal regions of this peptide are topologically partitioned to face the cytoplasmic and luminal sides of ER membranes, respectively, whilst its core hydrophobic region is spanning across membranes)[22-24]. Nonetheless, formal publication of this original work was maliciously delayed by a peer-reviewing scientist with only a similar competitive publication emerged during his assessment.

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Multi-level Micromechanical Model for Elastic Properties of Hybrid Fiber Reinforced Concrete

by Jiann-Wen Woody Ju, Member EUAS

Short Biography

Professor Jiann-Wen Woody JU *received his M.S. and Ph.D. degrees from the UC Berkeley. He is a senior Professor at* ***UCLA****, and served as the Department Chair of Civil and Environmental Engineering. Prof. Ju served as an Associate Editor for the ASME Journal of Engineering Materials & Technology, and for the ASME Journal of Applied Mechanics from 1995 to 2002. He is currently the* ***Editor-in-Chief*** *of the International Journal of Damage Mechanics, an Associate Editor of the ASCE J. of Nanomechanics and Micromechanics, and an Editorial Board member of the Acta Mechanica. He served as the ACI 446 Committee Chair. Prof. Ju received the 1991 Presidential Young Investigator Award from NSF and White House, 1991 Alfred Rheinstein Faculty Award from Princeton Univ., 1997 ASCE Walter Huber Civil Engineering Research Award, 1998 ASME Fellow Award, 2000 ACI-James-Instruments Award in NDE, 2006 ASCE Fellow Award, 2007 USACM Fellow Award, 2008 ACI Fellow Award, 2008-2009 Invited Chair Professor from University of Paris VI and ENS Cachan (France), 2008 Publication Award of Merit from the Structural Engineers Association, 2009-2012 Chang-Jiang Scholar Chair Professor (Ministry of Education, China), 2010 IACM Fellow Award, 2010 Kwang-Hua Chair Professor (Tongji University), 2011-2013 Tongji Univ. Chair Professor, National 1000 Talents Program (Short-Term) Distinguished Chair Professor (2013-present), Tongji University Distinguished Chair Professor (2013-present), Guangxi University Distinguished Chair Professor (2013-present), 2013 ICACM Award, and Honorary Distinguished University Professor from Southwest Jiaotong University (2015-present), 2018 ICDM-3 Lifetime Achievement Medal, and 2018 EU Academy of Sciences Member, etc. Prof. Ju has published more than* ***140*** *SCI-indexed scholarly journal papers. Furthermore, Prof. Ju's journal publications have been highly cited by the Web of Science (SCI); his* ***h-index*** *is currently* ***41*** *(Google Scholar). His research interests and research projects encompass structural engineering, structural mechanics, computational mechanics, computational damage, healing and fracture mechanics, micromechanics and nanomechanics of composites, multiscale material modeling, finite elements, biomechanics, computational geomechanics and geotechnical engineering, reliability, service life predictions, durability of concrete and cementitious composites, sulfate attack problems, environmental assessment and hazard, risk analysis and management, hazard mitigation, multiphase porous flow and transport, and wind-wave-bridge interactions and damage effects, etc.*

A multi-level micromechanical model for elastic properties of hybrid fiber reinforced concrete.

Yao Zhang, Zhi-guo Yan, J. Woody Ju, He-hua Zhu, Qing Chen

Construction and Building Materials 152 (2017) 804–817

Abstract

There is a demand for multi scale micromechanical models to disclose and analyze the effects of microstructure on macro mechanical properties of hybrid fiber reinforced concrete (HFRC).

This study involved presenting a multi-level micromechanical model that involves cement paste level, concrete level, and hybrid fiber reinforced concrete level to quantitatively predict the effective isotropic and elastic properties of HFRC under ambient temperature. For the purposes of homogenization, the volume fractions of different phases at different levels are determined by means of a modified Power's model. In the multi-level micromechanical model, hydration products of clinker, sand, coarse aggregate, and hybrid fiber are comprehensively considered. A homogenization stepping framework is presented to realize upscaling from microstructural properties to the effective elastic properties of a macrostructure for HFRC. Additionally, several substepping homogenizations are also presented to estimate the effective elastic properties of an equivalent medium with respect to the cement paste and hybrid fiber reinforced concrete. Comparisons with experimental data from extant studies are implemented level by level. Subsequently, the influences of aggregate, sand, fiber type, and hydration degree on the properties of HFRC are discussed based on a proposed multi-level micromechanical model. Finally, the mixture ratio of steel fiber and w/c are investigated with respect to the HFRC design to obtain anticipated elastic properties.

Elastoplastic damage micromechanics for continuous fiber-reinforced ductile matrix composites with progressive fiber breakage.

Y Wu and JW Ju

International Journal of Damage Mechanics 2017, Vol. 26(1) 4–28

Abstract

An elastoplastic damage micromechanical framework considering evolutionary fiber breakage is proposed to predict the overall material behaviors of continuous fiber-reinforced composites with ductile matrix under external loading. In the present work, we assume that the overall nonlinear behavior of a composite is primarily attributed to the plastic deformation in the matrix as well as the damage evolution due to fiber breakage. The effective elastoplastic deformations are governed by means of the effective yield surface derived from a representative microstructure with elastic fibers embedded in an elastoplastic matrix material. The matrix behaves elastically or plastically depending on the local stress, and the effective elastoplastic deformation obeys the associative plastic flow rule and isotropic hardening law. In addition, taking advantage of the eigenstrain due to fiber breakage together with a Weibull statistic model, the evolutionary fiber breakage mechanism is effectively predicted. Finally, the overall elastoplastic stress–strain responses are reached under the framework of micromechanics and damage mechanics. Comparisons between the proposed theoretical predictions and experimental data are performed to illustrate the capability of the proposed framework. In particular, the proposed model is employed to investigate the overall uniaxial and axisymmetric elastoplastic stress–strain responses of the continuous fiber-reinforced metal matrix composites. Studies of the initial yield surfaces at various damage levels are conducted as well.

An equivalent elastoplastic damage model based on micromechanics for hybrid fiber-reinforced composites under uniaxial tension.

Zhi-guo Yan, Yao Zhang, J Woody Ju, Qing Chen and He-hua Zhu

International Journal of Damage Mechanics 2019, Vol. 28(1) 79–117

Abstract

A micromechanics-based equivalent elastoplastic damage model for both notch-sensitive nd multiple cracking hybrid fiber reinforced composite is proposed in this study. In this model, the elastic modulus, first cracking strength, and ultimate strength are estimated based on micromechanics. To quantify strain after matrix cracks, a novel characteristic length is defined based on the damage mechanics. The effects of the fiber length, diameter and modulus, and interfacial bond stress on the characteristic length of hybrid fiber reinforced composite are presented. In order to avoid the difficulty of determining the traditional damage and plastic potential function, this model is developed from the behavior of single fiber at mesolevel to the response of hybrid fiber reinforced composite at macrolevel. Then the calculated results are verified with several published experimental results of fiber reinforced composites and hybrid fiber reinforced composite, including notch-sensitive cracking fiber reinforced composite, multiple cracking fiber reinforced composite, and multiple cracking hybrid fiber reinforced composite reinforced with two types of fibers (steel fiber and polyethylene fiber). A parametric study has been performed to investigate the effects of the fiber properties, including the fiber volume fraction, length, diameter, and interfacial bond stress, on the tensile performance of hybrid fiber reinforced composite reinforced with steel fiber-like and polyethylene fiber-like fibers. The results indicate that enhancement of the tensile performance can be achieved more effectively by improving the polyethylene fiber-like fiber than steel fiber-like fiber.

A novel multi-scale model for predicting the thermal damage of hybrid fiber-reinforced concrete.

Yao Zhang, J Woody Ju, Hehua Zhu and Zhiguo Yan

International Journal of Damage Mechanics 2019

Abstract

A multi-scale micromechanical model is proposed to predict the damage degree of hybrid fiber-reinforced concrete under or after high temperatures. The thermal degradation of hybrid fiber-reinforced concrete is generally composed of the damage of the cement paste caused by thermal decomposition and thermal incompatibility, the deterioration of aggregates and fibers, and the interfacial damage between aggregates and the matrix. In this multi-scale model, four levels of hybrid fiber-reinforced concrete structures are considered when the thermal damage degree is derived; namely, the equivalent calcium silicate hydrate (C–S–H) product level, the cement paste level, the concrete level, and the hybrid fiber-reinforced concrete level. At the cement paste level, thermal decompositions of C–S–H product and calcium hydroxide are taken into account. In addition, a dimensionless parameter of the crack density is introduced to represent the thermal cracking of the matrix. At the concrete level, the interfacial damage of aggregates is simulated by a spring–interface model, in which the interfacial parameters are assumed to be functions of temperature. Moreover, at the cement paste level and the hybrid fiber-reinforced concrete level, a substepping homogenization method is proposed to determine the effective properties. Comparisons between previously published experimental data and predictions and discussions illustrate the feasibility of the proposed multi-scale model in predicting thermal damage of concrete and hybrid fiber-reinforced concrete.

A stochastic micromechanical model for fiber-reinforced concrete using maximum entropy principle.

Qing Chen, Hehua Zhu, J. Woody Ju, Zhiguo Yan, ChanghongWang, Zhengwu Jiang

Acta Mech 229, 2719–2735 (2018)

Abstract

A stochastic micromechanical framework is presented to predict the probabilistic behavior of the fiber-reinforced concrete (FRC) using the maximum entropy principle. The FRC is represented as a multiphase composite composed of the aggregate, the interfacial transition zone, the bulk cement paste, and the fiber. The volume fractions of the different constituents are analytically calculated based on the material mix proportions and the aggregate grading. The multilevel homogenization schemes are presented to predict the material's effective properties considering the effects of the aggregate, the ITZ, and the fibers with the different shapes. By modeling the volume fractions and properties of constituents as stochastic, we extend the deterministic framework to stochastic to incorporate the inherent randomness of effective properties among the different specimens. The maximum entropy distribution is modified to estimate the probability density function of the material's properties using their different order moments. Numerical examples including the limited experimental validations, the comparisons with existing micromechanical models, the commonly used probability density functions, and the direct MonteCarlo simulations indicate that the proposed models provide an accurate and computationally efficient framework in characterizing the material's effective properties.

A novel damage model based on micromechanics for hybrid fiber reinforced cementitious composites under uniaxial compression.

Yao Zhang, J Woody Ju, Hehua Zhu, Qing Chen, Qinghua Guo and Zhiguo Yan

International Journal of Damage Mechanics 2018

Abstract

A novel damage model based on micromechanics is proposed for hybrid fiber reinforced cementitious composites under uniaxial compression. In this model, a multilevel homogenization method is presented to predict the overall elastic properties of hybrid fiber reinforced cementitious composites. To account for the contribution of microcracks on its macrocompliance under compression, hybrid fiber reinforced cementitious composite is considered equivalent to the microcrack-weakened solid, whose overall compliance consists of the compliance of the matrix and the additional compliance by sliding, propagating and kinking cracks. The bridging effects of hybrid fibers on restraining crack growth are simplified based on the reality that the average sliding displacement of microcracks is much less than the length of reinforcing fibers. The evolutional domains of microcrack growth under loads where the microcracks are sliding, propagating and kinking are discussed in detail. In addition, the weakening effects of fibers upon compressive behavior are captured by introducing two functions, which consider the influences of fiber
geometrical parameters, the microcrack density and the distance between two nearest microcracks with the same oriented angle. Simulation results by our evolutionary damage model render reasonable agreements with available experimental data of fiber reinforced cementitious composites and hybrid fiber reinforced cementitious composites with various fiber contents. The new micromechanical damage model would be beneficial to elucidating the strengthening and weakening mechanisms of hybrid fiber reinforcement.

Dreaming of No More Renal Dialysis

by Giuseppe Remuzzi, Member EUAS

Short Biography

Giuseppe Remuzzi completed his medical training at the University of Pavia in 1974 and then received specialty training in Haematology and Nephrology at the University of Milan in 1977 and 1980, respectively. From 1996 until 2013 he was Director of the public-private Department of Immunology and Transplant Medicine (a collaboration between the Ospedali Riuniti of Bergamo and the Mario Negri Institute) and from 1999 until 2018 he has also been Head of the Division of Nephrology and Dialysis. From 2011 until 2015 he was Director of the Department of Medicine of the Azienda Ospedaliera Papa Giovanni XXIII (formerly the Ospedali Riuniti) of Bergamo. In June 2015 he was nominated Chiara Fama Professor of Nephrology at the University of Milan. Alongside his clinical work in hospital, Prof. Remuzzi has dedicated himself to intense didactic and research activities. Since the Mario Negri Institute for Pharmacological Research opened its branch in Bergamo, Prof. Remuzzi has coordinated all of the research that takes place there, and since 1992 he has done the same for the Aldo e Cele Daccò Clinical Research Centre for Rare Diseases in Ranica, Bergamo. Since July 1st Professor Remuzzi has also taken on the role of Director of the the Mario Negri Institute. His main research interests include the causes of glomerulonephritis and the mechanisms of progression of kidney diseases. He has also conducted many studies in the field of transplant rejection. With an innovative approach (transplanting two kidneys from older donors into one recipient, after carefully evaluating the condition of the organs), his research has facilitated an increase in the number of transplants conducted. His most recent research concerns the possibility of regenerating tissues and creating organs in the laboratory using stem cells.

Prof. Remuzzi serves on editorial boards of numerous journals and is member of the International Advisory Board of The Lancet. He served as Editorial Board member of the New England Journal of Medicine from 1998-2013. In recognition of his achievements, he has been awarded in 1998 honorary memberships of the Association of American Physicians and the British Royal College of Physicians. In 2005 during the World Congress of Nephrology in Singapore he received the ISN Jean Hamburger Award. In 2007 he received during the annual American Society of Nephrology Congress in San Francisco the prestigious ASN John P. Peters Award and in 2011 he was awarded with the ISN AMGEN Award (World Congress of Nephrology: WCN 2011, Vancouver). In November 2011 he received the Third Edition of the International Award "Luis Hernando" assigned by the Iñigo Alvarez de Toledo Renal Foundation (FRIAT) in Madrid, Spain.

From June 2013 until March 2015 he was President of the International Society of Nephrology (ISN). During his tenure he created and launched the global 0by25 project, the goal of which is that "Nobody should die of preventable and treatable Acute Kidney Injury (AKI) by 2025".

In April 2018 he was awaded the "Lennox K. Black International Prize for Excellence in Medicine" at the Thomas Jefferson University in Philadelphia.

Prof. Remuzzi is the author of over 1450 publications in International medical journals and has written 16 books. He also regularly writes editorials for the Corriere della Sera newspaper.

Dreaming of No More Renal Dialysis

Giuseppe Remuzzi has a talent for making dreams come true. Recently made head of the Department of Immunology and Clinical Organ Transplantation in Bergamo's hospital, Italy—a joint private–public facility linking the Mario Negri Institute, Bergamo, and the hospital —Remuzzi has devoted much of his working

life to studying renal disease. Now, Remuzzi believes his dream of no more renal dialysis may soon be reality. 35 years ago, Remuzzi started the Mario Negri Institute in his home town of Bergamo, despite local opposition. The "Negri-Bergamo", which he has directed ever since, is an off-shoot of Italy's first non-profit research foundation which was created in 1963 in nearby Milan by Silvio Garattini. Before the inception of Negri-Bergamo, Remuzzi's group consisted of two dozen dedicated young scientists working together in a single room, known as the "metabolic cage", in Bergamo's hospital. On a visit to London, remembers Remuzzi, "I told Garattini that we can't go on like this, we must open a 'Mario Negri' in Bergamo". With Garattini's drive and Remuzzi's leadership an outstanding 170-scientist unit developed, in which basic and clinical research are interwoven in the common pursuit of turning bedside dreams into reality.

"During my medical studies in Pavia, I set up a student theatre", recalls Remuzzi. "This, I think I am still doing, since I believe coordinating research is not unlike directing plays." Arrigo Schieppati (head of the Rare Diseases Unit at Negri-Bergamo), one of Remuzzi's original aides-de-camp, agrees. Remuzzi is "a formidable generator of research hypotheses", he explains, "but he can also spot peoples' talents and assign the right role to the right person". Another researcher who was in at the start of the institute and remains with Remuzzi to this day—as indeed do most of his original colleagues—is Aricla Benigni, head of the Mediators Laboratory. "Remuzzi managed to get different people to work in different fields all converging on the same clinical problems, constantly transmitting his contagious enthusiasm and unconditioned dedication to the whole team", she explains.

Remuzzi studied humanities at school, then medicine at university, intending to fuse the two disciplines by becoming a psychoanalyst. But after qualifying as a physician, the first one in a family of marble artisans and sculptors, Remuzzi trained in haematology. His move into nephrology happened by chance when he filled a vacant nephrology position in Bergamo's hospital. "With Manuela Livio [a biologist] and our mentor Giovanni de Gaetano, I had been working on platelets, so what intrigued me was why uraemic patients bleed. But had it not been for Manuela, I would not be a researcher. We started together. She worked in the lab, I saw the patients. Sadly, Manuela died of leukaemia shortly after Negri-Bergamo was set up, an irreplaceable loss."

Remuzzi has long dreamed that one day renal dialysis will no longer be needed. Some years ago on a journey to Milan with colleague Tullio Bertani, now head nephrologist in Bergamo, the two doctors discussed the state of nephrology. "Nobody really knows what's going on here; the cause of glomerulonephritis and of most renal diseases is obscure; there is no way to stop their progression; and renal grafts are doing badly." To prevent patients deteriorating to a point where they needed dialysis, "we decided there was only one solution—research". Two main problems had to be tackled before the "no-more-dialysis" dream could be realised,

says Remuzzi. “Renaldisease progression had to be stopped and chronic graft rejection had to be blocked.”

Remuzzi believes that the dream is now within reach. 10 years of animal research at Negri-Bergamo showed that increased protein traffic across the glomeruli causes nephropathies to progress rather than vice versa. Moving into the clinic, the REIN study (ramipril efficacy in nephropathy)—his finest achievement so far, says Benigni—“showed that by limiting protein traffic we can halt renal disease progression in half the patients doomed to develop endstage renal failure”, notes Remuzzi, “And I expect more good news from the follow-up of REIN.” What about renal transplantation? “Immunosuppression carries unacceptable tox toxicity”, says Remuzzi. For example, cancer can be expected in all graft recipients whose grafts survive for more than 30 years. In 1990, other researchers achieved donor-specific immune tolerance in rats by doing intrathymic islet transplantation. “A year later”, Remuzzi notes, “we induced tolerance to the kidney by intrathymic glomerular transplantation in rats”, a process that allowed indefinite survival of renal grafts without immunosuppression. The concept of intrathymic tolerisation is now being tested in Pittsburgh, PA, USA on children receiving heart transplants.

While waiting for the results of this study, Remuzzi’s group is not dozing. Concerned by kidney donation shortages and deploring the current practice of discarding suboptimal donor kidneys, the team has shown that transplanting such kidneys in pairs is feasible and have set up an international effort to validate the approach. They are also transfecting immunomodulatory genes into grafts. This is a promising approach, says Remuzzi. “However, we don’t know how long the genes will stay there.” What we really need, he adds, is a way of preventing rejection that is “tolerable for the patient and affordable, even in the developing world”. With this in mind, his group has adopted a “renal sister centre” in La Paz, Bolivia, so that they can share their expertise with people in this poor region.

Remuzzi’s clinical interests are not limited to nephrology. He has a longstanding fascination for uncommon disorders. He quotes Garattini’s observation that “patients with rare diseases are more unfortunate than those with common disorders: they are less likely to find the right physician”. In 1993, Garattini and Remuzzi set up a clinical research centre for rare diseases in a villa near Bergamo. Here, explains Remuzzi, “we can gather more patients with a rare disease than specialists are likely to see in a lifetime. Patients and experts can stay here free of charge” while clinical research is done—another dream turned into reality.

Analysis of Three-Dimensional Atom-Probe Data by the Proximity Histogram

by David N. Seidman, Member EUAS

Short Biography

CURRENT POSITIONS

Walter P. Murphy Professor of Materials Science and Engineering, Northwestern University
Founding Director, August 2004, Northwestern University Center for Atom-Probe Tomography (NUCAPT)
Member of the National Science Foundation Funded Materials Research Science and Engineering Center
Co-Founder and Co-Chief Scientific Officer of NanoAl LLC, Illinois Science + Technology Park, 8025 Lamon Ave, Suite 446, Skokie, IL 60077 http://nanoal.com/: Founded June 2013 and sold on September 19th, 2018 to Braidy Industries, https://www.braidyindustries.com/about/

EDUCATION

Post-doctoral fellow, Cornell University, October 1964 to December 1965
Ph.D. Physical Metallurgy (major) and Physics (minor), University of Illinois at Urbana-Champaign, 1965
M.S. Physical Metallurgy, New York University, January 1962
B.S. Physical Metallurgy (major) and Physics (minor), New York University, 1960
Brooklyn Technical High School, Brooklyn, NY, 1952-1956, College Preparatory diploma with honors

PROFESSIONAL SOCIETIES

Member National Academy of Engineering, 2018
Member EU Academy of Sciences (EUAS), 2018
Honorary AIME Honorary Member Award 2014; nominated by the TMS (Minerals•Metals•Materials)
Fellow American Academy of Arts & Sciences, 2010
Fellow American Association for the Advancement of Science, 2014
Fellow American Physical Society, Division of Condensed Matter Physics, 1983
Fellow ASM International, 2005
Fellow Inaugural class of fellows, International Field-Emission Society, 2016
Fellow John Simon Guggenheim Memorial Foundation, 1980-81
Fellow John Simon Guggenheim Memorial Foundation, 1972-73
Fellow Materials Research Society, 2010
Fellow Microscopy Society of America, 2012
Fellow TMS (Minerals•Metals•Materials), 1997
Member Alexander von Humboldt Association of America
Member Böhmische Physical Society
Member New York Academy of Sciences

HONORS AND AWARDS

2019 A. Frank Golick Lecturer, Missouri University of Science & Technology, Department of Materials Science and Engineering
2019 ASM International Gold Medal award
2018 Member, National Academy of Engineering (NAE)
2018 Member, EU Academy of Sciences (EUAS)
2016 Fellow of the Inaugural Class, International Field-Emission Society (for atom-probe tomography, atom-probe field-ion microscopy, field-ion microscopy and their development and numerous applications to materials science and engineering)
2015 ASM International Edward DeMille Campbell Memorial Lectureship, presented at MS&T meeting, October 7th, 2015, Columbus, Ohio
2014 AIME Honorary Member Award; nominated by the TMS (Minerals•Metals•Materials)
2014 Fellow, American Association for the Advancement of Science
2012-2013 Sackler Lecturer, 2012-2013, of the Mortimer and Raymond Sackler Institute of Advanced Studies, Tel-Aviv University
2012 Fellow of Microscopy Society of America
2011 TMS (Minerals•Metals•Materials) Institute of Metals Lecture and the Robert Franklin Mehl Award for 2011
2010 Fellow of the American Academy of Arts & Sciences
2010 Fellow of the Materials Research Society
2010-2011 IBM Faculty Research Award
*2009 Structural Materials Division Symposium: Advanced Characterization and Modeling of Phase Transformations in Metals in Honor of David N. Seidman: TMS **(Minerals•Metals•Materials)** 2009 Annual Meeting, San Francisco, California; February 15th to 19th, 2009.*

2008	*David Turnbull Lecturer Award, Materials Research Society. Awarded, December 3rd, 2008: Boston MRS Fall meeting*
2006	*Albert Sauveur Achievement Award, ASM International*
2005	*Fellow of ASM International*
2001-2003	*National Science Foundation Creativity Extension Award*
2000	*Microscopy of Society of America award for Best Materials Papers appearing in Microscopy and Microanalysis, see publication numbers 218 and 219.*
1997	*Fellow of the TMS (Minerals•Metals•Materials)*
1996	*Walter P. Murphy Professor of Materials Science and Engineering at Northwestern University*
1993	*Max Planck Research Prize of the Max-Planck-Gesellschaft and the Alexander Von Humboldt Stiftung awarded jointly with the late Prof. Dr. Peter Haasen*
1993-2002	*Special Editions Editor and member of the Editorial Board of Interface Science (Kluwer Academic Publishers)*
1992	*Alexander Von Humboldt Stiftung Prize*
1988	*Teacher of the Year Award, Department of Materials Science & Engineering, Northwestern University*
1988	*Alexander Von Humboldt Stiftung Prize*
1984	*Fellow of the American Physical Society, Division of Condensed Matter Physics*
1982	*Chairman of the Physical Metallurgy Gordon Conference on the special topic of interfacial segregation*
1982	*Elected member of the Böhmische Physical Society*
1980-1981	*Lady Davis Visiting Professor, The Hebrew University of Jerusalem*
1980-1981	*Fellow of the John Simon Guggenheim Memorial Foundation*
1968-1977	*MITRE evaluative study of Materials Research Laboratory Programs (MTR 7764) rated my research program for the years 1968-1977 among the top twenty most highly rated major achievements sponsored by the National Science Foundation in the area of materials science.*
1978	*Lady Davis Visiting Professor, The Hebrew University of Jerusalem*
1972-1973	*Fellow of the John Simon Guggenheim Memorial Foundation*
1966	*Robert Lansing Hardy Gold Medal of the American Institute of Metallurgical Engineers [now the TMS (Minerals•Metals•Materials)]*
1959	*Tau Beta Pi, Engineering Honor Society, New York University*
1959	*Alpha Sigma Mu, Metallurgy Honor Society, New York University*
1955	*Order of the Arrow, Vigil rank, Boy Scouts of America*
1952	*Eagle Scout, Boy Scouts of America, February 15th, 1952*

O. C. Hellman, J. A. Vandenbroucke, J. Rüsing, D. Isheim, and D. N. Seidman, **"Analysis of Three-Dimensional Atom-Probe Data by the Proximity Histogram,"** *Microscopy and Microanalysis* **6**, 437-444 (2000). *Named Best Materials Paper published in Microscopy and Microanalysis in the year 2000*.

Abstract

The three-dimensional (3D) atom-probe technique produces a reconstruction of the elemental chemical identities and three-dimensional positions of atoms field evaporated from a sharply pointed metal specimen, with a local radius of curvature of less than 50 nm. The number of atoms collected can be on the order of one million, representing an analysis volume of approximately 20 nm x 20 nm x 200 nm (80,000 nm(3)). This large amount of data allows for the identification of microstructural features in a sample, such as grain or heterophase boundaries, if the feature density is large enough. Correlation of the measured atomic positions with these identified features results in an atom-by-atom description of the chemical environment of crystallographic defects. This article outlines a data compilation technique for the generation of composition profiles in the vicinity of interfaces in a geometrically independent way. This approach is applied to quantitative determination of interfacial segregation of silver at a MgO/Cu(Ag) heterophase interface.

E. A. Marquis and D. N. Seidman, **"Nanoscale Morphological Evolution of Al_3Sc Precipitates in Al(Sc) Alloys,"** *Acta Materialia* **49**, 1909-1919 (2001).

Abstract

Precipitation of the Al_3Sc ($L1_2$) phase in aluminum alloys, containing 0.1, 0.2 or 0.3 wt.% Sc, is studied with conventional transmission and high-resolution (HREM) electron microscopies. The exact morphologies of the Al_3Sc precipitates were determined for the first time by HREM, in Al-0.1 wt.% Sc and Al-0.3 wt.% Sc alloys. The experimentally determined equilibrium shape of the Al_3Sc precipitates, at 300˚C and 0.3 wt.% Sc, has 26 facets, which are the 6 {100} (cube), 12 {110} (rhombic dodecahedron), and 8 {111} (octahedron) planes, which is a Great Rhombicuboctahedron. This equilibrium morphology had been predicted by first principles calculations of the pertinent interfacial energies. The coarsening kinetics obey the $(time)^{1/3}$ kinetic law of Lifshitz-Slyozov-Wagner theory and they yield an activation energy for diffusion, 164±9 kJ/mol, that is in agreement with the values obtained from tracer diffusion measurements of Sc in Al and first principles calculations, which implies diffusion-controlled coarsening.

K. Knipling, D. C. Dunand, and D. N. Seidman, **"Criteria for Developing Castable, Creep Resistant Aluminum-Based Alloys – A Review,"** *Zeitschrift für Metallkunde* **97**, 246-265 (2006).

Abstract

We describe four criteria for the selection of alloying elements capable of producing castable, precipitation-strengthened Al alloys with high-temperature stability and strength: these alloying elements must (i) be capable of forming a suitable strengthening phase, (ii) show low solid solubility in Al, (iii) exhibit low diffusivity in Al, and (iv) retain the ability for the alloy to be conventionally solidified. With regard to criterion (i), we consider those systems forming Al_3M trialuminide compounds, with a cubic $L1_2$ crystal structure, which are structurally analogous to Ni_3Al (γ') in the Ni-based superalloys. Eight elements, clustered in the same region of the periodic table, fulfill criterion (i): the first Group 3 transition metal (Sc), the three Group 4 transition metals (Ti, Zr, Hf) and the four latest rare-earth elements (Er, Tm, Yb, Lu). Based on a review of the existing literature, these elements are discussed in terms of criteria (ii) and (iii), which satisfy the need for a precipitate phase in Al with slow coarsening kinetics, and criteria (iv), which is discussed based on the extant binary phase diagrams.

Z. Mao, C. K. Sudbrack, K. E. Yoon, G. Martin, and D. N. Seidman, **"The Mechanism of Morphogenesis in a Phase Separating Concentrated Multi-Component Alloy,"** *Nature Materials* **6**, 210-216 (2007).

Abstract

What determines the morphology of a decomposing alloy? Besides the well-established effect of the nucleation barrier, we demonstrate that, in a concentrated multi-component

Ni(Al,Cr) alloy, the details of the diffusion mechanism affect strongly the kinetic pathway of precipitation. Our argument is based on the combined use of atomic-scale observations, employing 3-dimensional atom-probe tomography (3-D APT), lattice kinetic Monte Carlo simulations, and the theory of diffusion. By an optimized choice of thermodynamic and kinetic parameters we first reproduce the 3-D APT observations, in particular the early stage transient occurrence of *coagulated precipitates*. We then modify the kinetic correlations among the atomic fluxes in the simulation, without altering the thermodynamic driving force for phase separation, by changing the vacancy-solute interactions, resulting in a suppression of coagulation. Such changes can only be quantitatively accounted for with nonzero values for the off-diagonal terms of the Onsager matrix, at variance with classical models.

Z. Mao, C. Booth-Morrison, C. K. Sudbrack, G. Martin, and D. N. Seidman, **"Kinetic Pathways for Phase Separation: An Atomic-Scale Study in Ni-Al-Cr Alloys,"** *Acta Materialia*, **60**(4), 1871–1888 (2012).

Abstract

The kinetic pathways involved in the formation of □'($L1_2$ structure)-precipitates during aging of concentrated Ni-Al-Cr alloys at 873 K, for three distinct alloy compositions, are studied experimentally by atom-probe tomography, and computationally with lattice kinetic Monte Carlo (LKMC) simulations, whose parameters are deduced from first-principles calculations of cohesive energies, and from experimental diffusion data. It is found that the compositional evolution of the γ'-precipitate phase does not follow the predictions of a classical mean-field model for coarsening of precipitates in ternary alloys. LKMC simulations reveal that long-range vacancy-solute binding plays a key role during the early stages of γ'-precipitation. With the aid of Monte Carlo techniques, with the same parameters as used in LKMC, we compute the diffusion matrix in the terminal solid-solutions and demonstrate that key features of the observed kinetic pathways are the result of kinetic couplings among the diffusional fluxes. The latter are controlled by the long-range vacancy-solute binding energies. It is concluded that, because it neglects flux couplings, the classical mean-field approach to phase separation, despite its many qualitatively correct predictions, fails to describe quantitatively the true kinetic pathways that lead to phase separation in concentrated metallic alloys.

Z. Sun, A. Tzaguy, O. Hazut, L. J. Lauhon, R. Yerushalmi, and D. N. Seidman, **"Self-Assembly of Ordered 1-D Metal Nanobead Arrays Within Nanowires via a Red-Ox-Induced Dewetting Mechanism,"** *Nano Letters*, **17**(12) 7478-7486 (2017).

Abstract

Metal nanoparticles are one of the most important candidates for plasmonic applications due to their tenability in morphology and structure. Bottom-up self-assembly of metal nanoparticles provides an important alternative complement to the traditional top-down lithography method and makes it possible to assemble structures with higher-order complexity, for example, nanospheres, nanocubes, and core-shell nanostructures. Herein we introduce a new methodology to assemble noble metal nanoparticles, including Au, Ag and AuAg alloy nanoparticles, within a germanium nanowire by oxidizing a shape-

confining metal-germanium nanowire hybrid-structure. The resulting structure is an array of equidistant metal nanoparticles with the same diameters, the so-called nanobead (NB) structure. We propose a mechanism wherein the noble metal first forms a metal-germanium eutectic liquid, which then migrates into the nanowire driven by a capillary force. Finally, because of the Plateau-Rayleigh instability of the liquid column, the liquid breaks-up into equidistantly distributed nanoparticles with approximately the same diameter, denoted a one-dimensional (1-D) dewetting mechanism. Atom-probe tomography and transmission electron microscopy are utilized to obtain the elemental distributions and morphology of the NBs, respectively, at every synthesis step for various synthesis parameters to understand and support the 1-D dewetting mechanism.

Z. Sun, C. Huang, J. Guo, J. Dong, R. F. Klie, L. J. Lauhon, D. N. Seidman, **"Strain-Energy Release in Bent Semiconductor Nanowires Occurring by Polygonization or Nanocrack Formation"** *ACS Nano*, **13**(3), 3730-3738 (2019).

Abstract

Strain is an important engineering degree of freedom in semiconductors that is used to modulate carrier mobility, tune the energy bandgap, and influence the growth morphology of heterostructures. Strain relaxation mechanisms in epitaxial thin-films and nanowires, including phase transformation, dislocation generation and motion, and cracking may degrade electronic properties including carrier lifetime and mobility. Investigations of strain release mechanisms are therefore necessary to understand device degradation and failure modes of pre-strained electronic devices and flexible electronics that undergo large strain during operation. Raman spectroscopy and electron microscopy and diffraction were used to identify strain-energy release mechanisms of bent diamond-cubic silicon and zinc-blende GaAs nanowires that were elastically strained at ambient temperature and then annealed to activate relaxation mechanisms. High temperature annealing of Si nanowires leads to nucleation of dislocations and the formation of grain boundaries, via glide and climb, which reduces the strain energy. For the first time, silicon nanowires were observed to undergo polygonization, which is the formation of polygon-shaped grains separated by grain-boundaries consisting of aligned edge dislocations. In contrast, GaAs nanowires release their strain-energy by forming nanocracks in the outer portion of a GaAs nanowire under tensile strain, and no polygonization is observed.

Towards Environmentally Benign Catalytic Processes

by Alfons Baiker, Member EUAS

Short Biography

***Present Position**: Professor emeritus at the Department of Chemistry and Applied Biosciences, Institute for Chemical and Bioengineering, ETH Zurich, Hönggerberg, HCI, CH-8093 Zurich, Switzerland,*

***Education and Employments:** 1971 Diploma Chemical Engineering (ETH); 1971 - 74 Ph.D.; 1974 - 76 Research Associate at ETH; 1976 - 78 Winner of International Younger Research Worker Interscheme, stays at several European Universities; 1978 - 80 Visiting Lecturer and Research Fellow Stanford University, California, USA (Prof. M.Boudart); 1980 Habilitation at ETH (Venia Legendi); 1980-1886 Lecturer and group leader; 1987 Honorary Professor; 1989 Associate Professor; 1990 Full Professor (ETH); 1993 - 95 Head of the Laboratory of Technical Chemistry; 1996 Visiting Professor at the University of California, Berkeley (USA) and at the Max-Planck Institute für Kohleforschung, Mülheim an der Ruhr (Germany); Since 2010 Professor emeritus at ETH; 2011-2015 Distinguished Adjunct Professor at King Abdulazis University (KAU), Jeddah, Saudi Arabia.*

An autobiography of Alfons Baiker is provided in the Festschrift on the occasion of his 65th birthday in the Journal of Physical Chemistry C, 2011, 115, 841-1374

***Research Interests:** Catalysis and Surface Chemistry; Chemical Reaction Engineering; Catalyst Design and Novel Catalytic Materials; Operando and in-situ Spectroscopy of Catalytic Surface Processes; Mechanisms and Kinetics of Catalytic Processes; Catalytic Syntheses of Chemicals from Carbon Dioxide; Environmental Catalysis; Catalysis for the Production of Fine Chemicals (Chemo-, Stereo- and Enantioselective Catalysis); Catalysis in Supercritical Fluids.*

***Other Activities:** Past and present Editorial or Advisory Board memberships: Journal of Catalysis; Catalysis Science & Technology, Journal of Molecular Catalysis A-General; ChemCatChem; Catalysis Letters; Applied Catalysis A-General; Applied Catalysis, B-Environmental; Catalysts and Catalytic Reactions; Catalysis Today; Chimia; Topics in Catalysis; Cattech; Research Letters in Chemical Engineering; Physical Chemistry Journal; Environmental Engineering Journal; Inorganic Chemistry Journal; Material Science Journal.*

Advisory Board Member of various congresses such as International Congress of Catalysis; World Congress of Oxidation Catalysis; International Symposium of Relation between Heterogeneous and Homogeneous Catalysis; International Symposium of Heterogeneous Catalysis for Fine Chemical. International Congress of Catalysis and Automotive Pollution Control.

Supervised over 100 Ph.D. students and over 80 postdoctoral researchers.

***Publications:** Over 900 publications in peer-reviewed journals, largely in catalysis and physical chemistry. 40'000+ citations, h-index 90 (Web of Science); 36 patents.*

***Awards and Honors:** Awards include the 1987 Ruzicka Award of Chemistry of the Board of the Swiss Federal Institutes (1987); Award of the Canadian Society for Chemical Engineering for outstanding work in Chemical Engineering (1987); Several Lectureships and best paper awards. "Karl Ziegler Visiting Professor" at Max-Planck Institute, Germany (1996); In 2006 he was ranked by ISI Web of Science (Thomson-Reuter) to belong to 0.5% top most cited scientists in the field of Chemistry in the past two decades.*

Research Achievements

The research of Baiker's group is highly interdisciplinary, including catalysis, surface science and chemical reaction engineering. Major contributions have been made in: Catalyst design and novel catalytic materials; Catalyst characterization, operando and *in-situ* spectroscopy of catalytic surface processes; Environmental catalysis; Catalytic syntheses of fine chemicals; Asymmetric catalysis and application of supercritical fluids in catalysis.

Catalyst Design and Novel Catalytic Materials

Our group has advanced the use of special techniques of solid-state chemistry, particularly molecular design concepts for developing novel catalytic materials. Supported metal catalysts with unique structural and chemical properties were prepared from glassy metal alloys for various reactions. Using underpotential deposition we developed useful methods for the *controlled deposition of heavy metal atoms* on supported noble metal catalyst. These methods provide a powerful tool for optimizing the active metal ensemble size and thereby the selectivity of supported metal catalysts. Efforts towards the synthesis of *ultrafine gold particles* suitable for catalysis afforded an efficient chemical route to gold clusters with mean diameter of 1.5 nm. We were among the first researchers who prepared *layer-type metal oxide catalysts by selective grafting* of suitable metal organic precursors, from liquid and gas phases, onto functionalized support materials. Other materials in our focus are *aerogels*. Various novel aerogels oxides, mixed oxides as well as metal/oxide systems with interesting catalytic potential have been synthesized and characterized. Basic studies using NMR and vibrational spectroscopy have provided new insight in the relationship between sol-gel and supercritical drying parameters and the structure of the resulting aerogels. Systematic studies on the platinum-cinchona system used for the enantioselective hydrogenation of α-ketoesters have uncovered many important features of this complex catalytic system. The knowledge gained on the mechanism of enantio-differentiation has led to the exciting opportunities of utilizing molecularly engineered chiral modifiers and the originally narrow range of substrates, which could be transformed enantioselectively on solid catalysts has significantly been extended.

Catalyst Characterization, Operando and in-situ Spectroscopy

A quantitative model that describes the interdependence of experimental conditions and peak shift in *Temperature programmed reduction* (TPR) has been developed and a criteria has been derived which allows to adjust the experimental parameters to achieve optimum sensitivity in TPR. *Pulse thermal analysis* (PTA) has been pioneered in our laboratory and applied for a variety of investigations. Special emphasis has been devoted to the development of methods for investigating *catalytic liquid-solid interfaces.* These methods, include *in-situ and operando Attenuated total reflection infrared* (ATR-IR) spectroscopy**,** *Polarization modulation-infrared reflection-adsorption spectroscopy (PM-IRRAS),* enabling simultaneous monitoring of the surface and gas- or liquid phase species**,** and *in-situ X-ray absorption spectroscopy* (XAS). A variety of sophisticated spectroscopic reactor cells have been developed for the investigation of gas-liquid-solid-interfaces under reaction conditions, including high pressure cells for the study of reactions in supercritical media. *ATR-modulation excitation spectroscopy* (ATR-MES) with phase sensitive detection has been established enabling the possibility to discriminate static and dynamic surface species. Criteria have been given that are essential for the design of reactor cells for *in-situ* studies where the elucidation of structure-activity relationships is targeted. These studies, which often have been combined with video-monitoring of the phase behavior, brought interesting new molecular insight into a variety of liquid-solid interfaces, including chirally modified metals, mixed oxides and organometallic complexes immobilized on functionalized silica.

Environmental Catalysis

The selective catalytic reduction of nitrogen oxides (SCR), oxidation of carbon monoxide, synthesis of chemicals from CO_2, partial oxidations, coupling and combustion of methane, and lean-burn engine and hybrid engine exhaust catalysis have been in our focus in this research area. Studies on *the selective catalytic reduction of NO* embraced its reaction mechanism and the surface structure of the vanadia, molybdena and chromia based catalysts. Using *in-situ* diffuse reflectance spectroscopy combined with mass spectroscopy and thermal desorption, the surface sites relevant for SCR were uncovered. With vanadia-based catalysts, the SCR activity was found to depend on the fraction of Brønsted-bound ammonia, which correlates with the vanadia surface concentration. To investigate the kinetics of SCR at very low reactant concentration (10^{-9} ppm), positron-emitting ^{13}NO molecules produced with a cyclotron were used. The measuring technique based on this short-lived radio active isotopes expands the accessible range of reactants by more than 11 orders of magnitude, and so opens the possibility of studying surface reaction kinetics in a totally new concentration regime. The understanding of the *structure sensitivity of SCR* observed over vanadia and chromia based SCR-catalysts has let to structurally optimized SCR catalysts based on vanadia and amorphous chromia. Another important topic of our group was the *utilization of carbon dioxide for the synthesis of value-added products*. Various aspects of the mechanism of these reactions were uncovered using vibrational spectroscopies and other techniques. The gained information together with the knowledge on amination reactions existing in the group, has led to the direct catalytic synthesis of aliphatic amines starting from CO_2, NH_3 and H_2. Later the potential of carbon dioxide as a C_1-building block in chemical synthesis has been demonstrated on various examples, including formylation of amines and the synthesis of organic carbonates. Studies on the *oxidation of carbon monoxide* have led to structurally and chemically optimized CO oxidation catalysts useful for low temperature applications. Research on the *partial oxidation of methane* revealed the relevance of surface and gas phase reactions for the selectivity to methanol. Palladium/zirconia catalysts highly active for methane combustion and selective for the production of synthesis gas were prepared by *in-situ* activation of glassy palladium zirconium alloys. In the field of *auto exhaust catalysis* our group discovered that several catalysts including Cu-ZSM-5 and alumina-based catalysts, which have been suggested to be suitable for lean burn- and diesel engine exhausts, can produce significant amounts of harmful HCN and HNCO. The formation of this harmful species has been overlooked by previous investigators dealing with these catalyst systems. Iridium-based catalyst were shown to possess interesting potential for auto exhaust catalysis. More recent work focused on *NO_x storage reduction (NSR) catalysts*. Systematic studies revealed that various Ba-containing species exist on the Pt-Ba/Al_2O_3 surface that show different efficiency in NO_x storage. The control of the population of these Ba-species was shown to be essential for optimal storage behavior.

Fine Chemicals Synthesis

Our research in fine chemical catalysis has enriched three important areas: chemoselective and enantioselective hydrogenation, partial oxidations, and aminations.
By systematic studies on *enantiodifferentiating heterogeneous Pt-cinchona alkaloid catalysts* used for the chiral hydrogenation of α-ketoesters our group has significantly advanced the knowledge on these complex catalytic systems. These investigations have

led to the design of promising new enantio-differentiating catalysts based on synthetic amino-alcohol type modifiers. The advantage of these modifiers is that a molecular engineering of both the stereogenic center as well as the anchoring group can be achieved, in contrast to the classical natural cinchona type modifiers. This opportunity has extended the narrow scope of substrates that can be transformed enantioselectively. First continuous enantioselective hydrogenation on solid catalysts was reported by the Baiker group. Fundamental experimental and theoretical studies have brought new insight into the functioning of these catalytic systems and uncovered phenomena such as the nonlinearity and switch of enantiodifferentiation observed with chirally modified metal surfaces. Extensive studies of the mechanism of mild *partial oxidations in the liquid phase* with air as oxidizing agent, using electrochemical methods and *in-situ* spectroscopy, such as ATR-IR and XAS, uncovered several new aspects of the reaction mechanism, which finally resulted in the design of more selective catalysts. *In-situ* catalyst potential measurements were used to gain information about the working state of the catalyst and for controlling the oxygen flux to the catalytic surface. Based on this concept high molecular weight and heat sensitive reactants such as alcohols and carbonyl compounds could be oxidized selectively using air as oxidant. Another field in oxidation catalysis, which was in the focus of our group is the *catalytic epoxidation*. We showed that amorphous titania-silica mixed oxide aerogels possess outstanding properties for the epoxidation of bulky olefins with alkylhydroperoxides as oxidants. Furthermore, important aspects of the reaction mechanism and catalyst tuning have been uncovered. Our early studies on the *amination of alcohols* have answered several important questions concerning this industrially important reaction. Aspects covered were catalyst design, mechanism, kinetics, and reaction engineering. Based on this knowledge new more economic continuous amination processes, which do not require high pressure were developed.

Catalysis in Supercritical Fluids

The potential of *supercritical fluids as reaction media* has been in our focus during several years. Fundamental aspects investigated embrace mass transfer of dense fluids entrapped in pores and the phase behavior in multicomponent reaction mixtures involving supercritical fluids. Supercritical carbon dioxide has been explored as an environmentally benign solvent in a variety of reactions, including catalytic chemoselective and enantioselective hydrogenations and later aerobic oxidations. Tuning of the properties of supercritical carbon dioxide by applying small amounts of co-solvents allowed to reach reaction rates in the oxidation of alcohols by air that are more than order of magnitude higher than those achieved with conventional solvents. *In-situ* ATR-studies of the catalytic fluid-solid interface combined with transmission IR studies of the bulk liquid phase brought new insight into the crucial role of the phase behavior and molecular interactions occurring under high pressure conditions. These studies clearly revealed that a profound understanding of the phase behavior, molecular interactions in the dense liquid phase as well as at the catalytic fluid-solid interface is necessary for proper exploitation of supercritical fluids as reaction media. Particularly interesting is the application where *supercritical carbon dioxide acts simultaneously as reactant and reaction medium*. Supercritical carbon dioxide has been used for the formylation of various amines with high efficacy. More recently this strategy of utilizing carbon dioxide for chemical synthesis has been successfully extended to the catalytic synthesis of organic carbonates.

Materials Science of Metastable Materials: Processing for Properties

by Jürgen Eckert, Member EUAS

Short Biography

Jürgen Eckert obtained his Ph.D. (German: Dr.-Ing.) in Materials Science and Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany in 1990. During collaborative research work with the Siemens Research Laboratories in Erlangen, he started research on the formation of amorphous and quasicrystalline alloys through interdiffusion, and subsequently extended it during a two and a half year postdoctoral stay at the California Institute of Technology. There he worked on the formation of nanocrystalline alloys via mechanical alloying. After a short break in industry, he moved to the Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, one of the leading Materials Research Science Centers in Germany. From 1996 until 2003 he was the Head of the Department Metastable and Nanostructured Materials at IFW Dresden, before he became Full Professor for Physical Metallurgy at TU Darmstadt. In 2006 he was appointed Director of the Institute for Complex Materials at IFW Dresden, and concurrently held the Chair for Synthesis and Analysis of Materials at Dresden University of Technology (TU) Dresden. In 2013/2014 he served as the Scientific Director of IFW Dresden. In 2015 he moved to Austria as Chair Professor of Materials Physics at Montanuniversität Leoben, and Director of the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences. He also held an Adjunct Professor Position at Michigan Technological University, Houghton, USA between 2002 and 2005, and was a Visiting Professor at University of Vienna, Austria at the Institute of Physics, Physics of Nanostructured Materials (2009 / 2010 / 2012).

He is an international expert in the field of metastable materials and has published more than 1100 papers in archival journals (h-index: 76 (WoS), more than 29.000 citations). He also published more than 150 conference papers, 18 book chapters, edited 6 books, conference proceedings and journal issues, and holds more than 20 patents.

Jürgen Eckert was honored as Dr. honoris causa (Dr. h.c.) by the Slovak University of Technology in Bratislava, Slovak Republic (2012), and received the prestigious Gottfried Wilhelm Leibniz Award of the German Research Foundation (2009), the highest Science Prize and scientific honor in Germany. Other honors include the DGM-Prize 2014 of the German Materials Research Society, an ERC Advanced Grant of the European Research Council (2013), the ISMANAM Senior Scientist Award (2012), the Hsun Lee Lecture Award of the Chinese Academy of Sciences (2006), the Georg-Sachs-Prize of the German Materials Research Society and the Austrian Metal Industry (1997), and the FEMS Materials Science and Technology Prize of the Federation of European Materials Science Societies (FEMS) in 1997. In addition, he received the Young Scientist Award of the German Materials Research Society (1994), and the ISMANAM Young Scientist Award (1997). He is a corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences (2017), a Member of the EU Academy of Sciences (2018) and has been elected to the class of 2018 MRS Fellows of the Materials Research Society, USA (2018).

Jürgen Eckert's research fields and scientific interests include phase formation, processing and structure-property correlations of metastable materials processed under non-equilibrium conditions; processing of materials by mechanical alloying/milling; structural and functional materials and metal matrix composites with particular emphasis on solidification fundamentals; rapid solidification processing; additive manufacturing techniques; biocompatible, magnetic and superconducting materials, and materials for energy applications and energy harvesting (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen storage) and thin film systems for flexible

electronics; solidification of metal matrix composites; mechanical and electrochemical properties of bulk materials, coatings and surfaces; biologically inspired far-from-equilibrium materials and architected structures; mathematical modelling of advanced materials and processes.

Over the years, Jürgen Eckert and his team have provided sustained contributions to research on metastable advanced high performance materials. Early work was devoted to work in the field of glass and quasicrystal formation in metallic systems, and fundamental observations on the development of nanoscale grain sizes in metallic materials. Later on the focus shifted to the development and property optimization of (Zr-, Ti-, Al-, Fe-, Mg-base) bulk metallic glasses (to mention a few) and their composites. In this field the work concentrated on developing plastically deformable bulk metallic glasses and composites through a synergistic approach by understanding how atomic scale structures, microstructural features and stress, plus processing-induced heterogeneities determine the mechanisms of plastic deformation on different length scales such as to overcome the otherwise unavoidable brittleness of glassy materials. Subsequently, this work developed into areas beyond metallic glasses creating new strategies for the design, synthesis and characterization of intrinsic length-scale modulation and phase transformations under highly non-equilibrium conditions. This concept defined new routes for creation of tailored nanostructured or ultrafine-grained structural and functional materials based on scale-bridging intelligent hybrid structures. Accordingly, this work expanded into high-strength lightweight applications, hard and soft magnetic materials, porous bulk materials and hybrid structures for biomedical applications, materials for energy applications (metals, oxides, hierarchical carbon structures), and also touched on surface modification and development of architected gradient structures. Some key publications in this area include:

- S. Pauly, S. Gorantla, G. Wang, U. Kühn, J. Eckert, "Transformation-Mediated Ductility in CuZr-Based Bulk Metallic Glasses", *Nature Mater.* 9, 473 (2010)
- J. Das, M.B. Tang, K.B. Kim, R. Theissmann, F. Baier, W.H. Wang, J. Eckert, ”Work Hardenable” Ductile Bulk Metallic Glass", *Phys. Rev. Lett.* 94, 205501 (2005)
- H. Guo, J. Eckert, W. Löser, L. Schultz, "Novel Ti-Base Nanostructure-Dendrite-Composite with Enhanced Plasticity", *Nature Mater.* 2, 33 (2003)
- Z.F. Zhang, J. Eckert, L. Schultz, "Difference in Compressive and Tensile Fracture Mechanisms of $Zr_{59}Cu_{20}Al_{10}Ni_8Ti_3$ Bulk Metallic Glass", *Acta Mater.* 51, 1167 (2003)
- J. Eckert, J.C. Holzer, C.E. Krill III, W.L. Johnson, "Structural and Thermodynamic Properties of Nanocrystalline fcc Metals Prepared by Mechanical Attrition", *J. Mater. Res.* 7, 1751 (1992)
- J. Eckert, L. Schultz, E. Hellstern, K. Urban, "Glass-Forming Range in Mechanically Alloyed Ni-Zr and the Influence of the Milling Intensity", *J. Appl. Phys.* 64, 3224 (1988)

Jürgen Eckert’s recent research activities after his move to Leoben focus on the development and application of methods for in-depth *in situ* and in operando investigation of phase transformations and structure-property correlations using local probes and high resolution techniques for structure characterization and imaging of local structures, chemical compositions and interaction of nanoscale objects with external fields and stimuli (e.g. mechanical, thermal, electrical, magnetic fields). The vision behind this approach is to create and test tailored biologically inspired far-from-equilibrium materials, hierarchical structures and correlated systems *in situ*, for example in a microscope or through flash annealing at extreme heating and cooling rates. This allows controlling the desired material

structure and additionally enables direct observation of the effect of structure on physical or mechanical properties. An example for such an attempt is the *in situ* design and testing of glassy metallic structures containing heterogeneities on different length-scales to overcome their intrinsic brittleness. These heterogeneities can be induced through different stimuli, for example a heat source, a laser, an ion or an electron beam. To study the deformation at the nanoscale, *in situ* tests are carried out within a transmission electron microscope or by using highly focused local probes at synchrotron beamlines. The concept of *in situ* design and testing is applicable to bulk structures and thin film systems and to a wide range of materials, and is therefore expected to open a new research avenue for creating materials with unique properties by design. Some very recent publications in this area include:

- B. Sarac, Y. P. Ivanov, A. Chuvilin, T. Schöberl, M. Stoica, Z. Zhang, J. Eckert, "Origin of Large Plasticity and Multiscale Effects in Iron-Based Metallic Glasses", *Nature Commun*. 9, 1333 (2018).
- C. Gammer, C. Ophus, T.C. Pekin, J. Eckert, A. Minor, "Local Nanoscale Strain Mapping of a Metallic Glass During In-Situ Testing", *Appl. Phys. Lett.* 112, 171905 (2018).

The long range perspective of these approaches and experiments is to further advance the understanding of structure-property correlations for hierarchically modulated structures and hybrid systems over a variety of different length-scales under highly non-equilibrium conditions. The goal is to gain a descriptive and quantitative picture of phase formation, transformation, dynamics and property design under extreme conditions, such as ultra-fast heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimulus. This promises to open new avenues for nanoscale structure formation in architected materials with unique functionality. For this purpose, state-of-the-art techniques from the fields of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and also structure-biological mimetic techniques and generative manufacturing are used to generate an atomic structural – functional understanding of the properties, performance and correlation of hierarchical thin film structures and membranes, tailored interface structures, nano- and multiscale hybrid systems and tailored “lattice materials”. But not only the basic fundamental mechanisms of structure formation and property development are of interest, but also the question how the findings can be transferred to applications in areas like MEMS/NEMS devices, sensors and actuators, energy storage or harvesting, or biocompatible (biodegradable) materials for personalized medical implants and medical devices.