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EUAS**

***EU ACADEMY
2016 ANNUAL REPORT***

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New Generation Spacecraft with Laser Engines by Universal Mechanics A Theory for the Nobel prize ?

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 of several Academies in USA.

For the design of the new generation spacecraft of any speed, the sophisticated theory of “**Universal Mechanics**” is proposed. The modern theory of “*Universal Mechanics*” consists of the combination of the theories of “*Relativistic Elasticity*” and “*Relativistic Thermo-Elasticity*”. Thus, according to the above theories there is a considerable difference between the absolute stress tensor and the stress tensor of the airframe even in the range of speeds of 50,000 km/h. Besides, for bigger speeds of the absolute spacecraft, like $c/3$, $c/2$ or $3c/4$ (c =speed of light), then the difference between the two stress tensors is very much increased. Hence, for the new generation spacecraft with very high speeds, the relative stress tensor will be therefore very much different than the absolute stress tensor. Also, for velocities near the speed of light, then the values of the relative stress tensor are very much bigger than the corresponding values of the absolute stress tensor. Such new generation spacecraft will be moving by using laser engines.

The theory of “*Relativistic Elasticity*” is a combination between the theories of “Classical Elasticity” and “Special Relativity” and results in the “**Universal Equation of Elasticity**”. Furthermore, the theory of “*Relativistic Thermo-Elasticity*” is a combination between the theories of “Classical Thermo-Elasticity” and “Special Relativity” and results in the “**Universal Equation of Thermo-Elasticity**”. The “structural design” of super speed vehicles requires the consideration of mass pulsation and energy-mass interaction at high velocity space-time scale, as the relative stress intensity factors are different than the corresponding

absolute stress intensity factors. Such theory results in the "*Universal Stress Intensity Factors*". Thus, the "*Universal Equation of Elasticity*", the "*Universal Equation of Thermo-Elasticity*" and the "*Universal Stress Intensity Factors*" are parts of the general theory of "*Universal Mechanics*".

The scope by the International Space Agencies is to achieve in the future, a new generation spacecraft moving with very high speeds, even approaching the speed of light. How far could be this future ? According to current author's research such future could be much closer than everybody believes. For the new generation spacecraft the relative stress tensor will be much different than the absolute stress tensor and so special solid should be used for the construction of the future spacecraft.

Besides, in order the future spacecraft to achieve very high speed, even approaching the speed of light, then such new generation spacecraft should be moving by using laser engines. Laser is light and so their speed is the speed of light. Consequently, the use of laser engines for the future spacecraft would be the best device.

Consider the state of stress at a point in the stationary frame S^0 , defined by the following symmetrical stress tensor: (Fig.1)

$$\sigma^0 = \begin{bmatrix} \sigma_{11}^0 & \sigma_{12}^0 & \sigma_{13}^0 \\ \sigma_{21}^0 & \sigma_{22}^0 & \sigma_{23}^0 \\ \sigma_{31}^0 & \sigma_{32}^0 & \sigma_{33}^0 \end{bmatrix} \tag{1}$$

where:

$$\sigma_{21}^0 = \sigma_{12}^0, \sigma_{31}^0 = \sigma_{13}^0, \sigma_{32}^0 = \sigma_{23}^0 \tag{2}$$

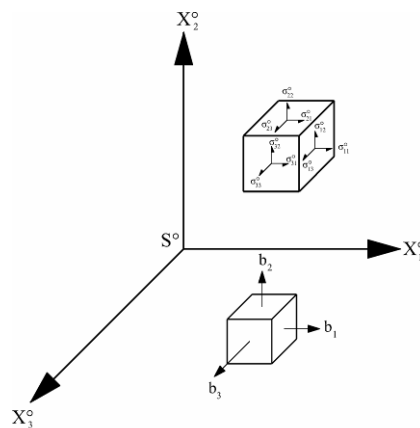


Fig. 1 The state of stress σ_{ik}^0 in the stationary system S^0 .

In addition, we consider an infinitesimal face element df with a directed normal, defined by a unit vector \mathbf{n} , at definite point p in the three-space of a Lorenz system. The matter on either side of this face element experiences a force which is

proportional to df .

Thus, the force is valid as:

$$d\boldsymbol{\sigma}(\mathbf{n}) = \boldsymbol{\sigma}(\mathbf{n}) df \tag{3}$$

The components $\sigma_i(\mathbf{n})$ of $\boldsymbol{\sigma}(\mathbf{n})$ are linear functions of the components n_k of \mathbf{n} :

$$\sigma_i(\mathbf{n}) = \sigma_{ik} n_k, \quad i, k = 1, 2, 3 \tag{4}$$

in which σ_{ik} is the elastic stress tensor, also called as the relative stress tensor, in contrast to the space part σ_{ik}^0 of the total energy-momentum tensor T_{ik} , referred as the absolute stress tensor (Fig. 2).

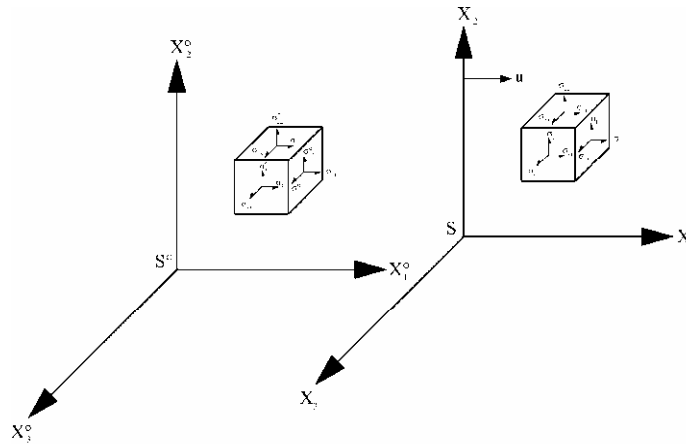


Fig. 2 The state of stress σ_{ik}^0 in the stationary system S^0 and σ_{ik} in the airframe system with velocity u parallel to the x_1 - axis.

Besides, the connection between the absolute and relative stress tensors is defined as:

$$\sigma_{ik}^0 = \sigma_{ik} + g_i u_k, \quad i, k = 1, 2, 3 \tag{5}$$

where g_i are the components of the momentum density \mathbf{g} and u_k the components of the velocity \mathbf{u} of the matter.

The relative stress tensor gives the **Universal Equation of Elasticity**:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \begin{bmatrix} \sigma_{11}^0 & \gamma \sigma_{12}^0 & \gamma \sigma_{13}^0 \\ \frac{1}{\gamma} \sigma_{21}^0 & \sigma_{22}^0 & \sigma_{23}^0 \\ \frac{1}{\gamma} \sigma_{31}^0 & \sigma_{32}^0 & \sigma_{33}^0 \end{bmatrix} \tag{6}$$

where γ is given by:

$$\gamma = 1/(1 - u^2/c^2)^{1/2} \tag{7}$$

with c the speed of light.

Consequently, “*Universal Mechanics*” gives the complete theory of mechanics for the whole universe. Then the theories of Special and General Relativity, as were proposed by Albert Einstein are completed for the whole universe by “*Universal Mechanics*”, as proposed by current author. Hence, by the current author is completed the theory of Albert Einstein for the whole universe regarding mechanics behavior. ***So, this theory could be nominee for a Nobel prize in physics.***

Table 1 shows the values of γ of relativity theory for some arbitrary values of the velocity u of the moving aerospace structure, where c is the speed of light (300,000 km/sec):

Table 1

Velocity u	$\gamma = 1/\sqrt{1 - u^2/c^2}$	Velocity u	$\gamma = 1/\sqrt{1 - u^2/c^2}$
50,000 km/h	1.000000001	0.800c	1.666666667
100,000 km/h	1.000000004	0.900c	2.294157339
200,000 km/h	1.000000017	0.950c	3.202563076
500,000 km/h	1.000000107	0.990c	7.088812050
10E+06 km/h	1.000000429	0.999c	22.36627204
10E+07 km/h	1.000042870	0.9999c	70.71244596
10E+08 km/h	1.004314456	0.99999c	223.6073568
2x10E+8 km/h	1.017600788	0.999999c	707.1067812
c/3	1.060660172	0.9999999c	2236.067978
c/2	1.154700538	0.99999999c	7071.067812
2c/3	1.341640786	0.999999999c	22360.67978
3c/4	1.511857892	c	∞

From Table 1 follows that for small velocities 50,000 km/h to 200,000 km/h, the absolute and the relative stress tensors are nearly the same. On the other hand, for bigger velocities like $c/3$, $c/2$ or $3c/4$ (c = speed of light), the variable γ takes values more than the unit and thus, relative stress tensor is very different from the absolute one. Additionally, for values of the velocity for the moving structure near the speed of light, the variable γ takes bigger values, while when the velocity is equal to the speed of light, then γ tends to the infinity.

For the design of the new generation spacecraft the “*Universal Stress Intensity Factors*” are further used. Thus, as was shown by the current author, the relative first and third mode stress intensity factors are the same for both stationary and moving frames, while the relative second mode stress intensity factor is much different in the above frames. All the relative stress intensity factors (first, second and third) are important for the fracture mechanics analysis of the future spacecraft, as for their fracture mechanics analysis a combination of all the three intensity factors should be used.

Structural Integrity of Load Bearing Components

by Ashok Saxena, Member EUAS



Short Biography

Dr. Ashok Saxena currently serves as the Provost and Vice-Chancellor of Academic Affairs at the University of Arkansas in Fayetteville overseeing the University's 200+ academic programs, 1500 faculty and 26,500 students. Previously, he served as the Dean of Engineering and the Raymond and Irma Giffels' Chair and the Head of the Biomedical Engineering Department at the University of Arkansas.

Dr. Saxena previously held the position of Regents' Professor and Chair 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. As their primary research advisor, he has mentored over 60 MS, doctoral and post-doctoral students.

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 awards and recognitions include the George Irwin Medal (1992) from the American Society for Testing and Materials (ASTM) for his pioneering contributions to creep fracture mechanics, the ASTM Award of Merit and Fellow (1994), Fellow of ASM International (1996), Georgia Tech Outstanding Research Author Award (1993) and the Fracture Mechanics Medal from ASTM in 2009. He was the recipient of the Wohler Fatigue Medal from the European Structural Integrity Society (ESIS) in 2010. He is the author/co-author/editor of eight books and over 250 research publications. In 2016, he became a member of the European Academy of Sciences.

We understand the catastrophic consequences of structural failures and that sometimes it is unavoidable, even if it occurs infrequently, because the factors involved in predicting it are complex and not fully understood. Since the 1960s, the developments in fracture mechanics and the associated analytical and experimental techniques have contributed immensely to our ability to avoid structural failures. New predictive analytical tools have been developed that have vastly improved our understanding of how cracks or crack-like defects in structural components that may escape detection, propagate and can potentially cause fracture. A large fraction of failures in structural components occur due to pre-existing defects, or defects that

initiate rapidly from clusters of nonmetallic inclusions, or from other imperfections such as casting, forging, and welding defects. However, several defects also lie dormant in the components and pose no threat of fracture. In assessing structural integrity we are interested in both types of defects, one that can potentially cause fracture, and those that are benign. Fracture mechanics provides an analytical framework for a comprehensive methodology for predicting the potential for fracture in components by considering: (i) the magnitude and distribution of applied stresses; (ii) the resistance to fracture and crack growth of the material from which the component is made; and (iii) the size, location, and geometry of defects in the component. This approach is also capable of considering the influence of service environment. Some applications of this analytical methodology include,

- accurate methods for designing new components that are fracture resistant,
- assessment of structural integrity of components when design changes are made,
- standardization of fracture test methods to determine relevant material properties to aid materials selection,
- prediction of remaining life of expensive components with life extension as a goal,
- estimation of inspection intervals or specification of inspection criteria as part of good maintenance practice, and
- fully understand field failures and their cause if and when they occur, so that future failures can be prevented.

Some examples from our recent work are briefly described.

Prognostics of High Temperature Component Reliability

Figure 1 shows a schematic diagram of the various elements of a methodology for prognostics of high temperature component reliability. They include the use of constitutive equations that consider the nonlinear and time-dependent aspects of deformation, and crack formation and crack growth models under high temperature conditions. The models must be able to account for complex conditions consisting of low frequency cyclic stress associated with thermal and mechanical loads generated during startup and shutdown, sustained stress resulting from centrifugal loading and aerodynamic loads during steady-state operation leading to creep conditions, and damage phenomena in high temperature materials under conditions of creep, oxidation, fatigue, and the synergistic effects of creep-fatigue-oxidation.

Our research has focused on several aspects of the methodology represented in Fig. 1 consisting of the following areas:

- Creep Crack Growth
 - Creep Crack Growth in Creep-Ductile Materials
 - Creep Crack Growth in Creep-Brittle Materials
 - Creep Crack Test Methods (ASTM Standard E1457)
- Creep-fatigue Crack Growth
 - Creep-fatigue Crack Growth in Creep-brittle Materials
 - Creep-fatigue Crack Growth in Creep-Ductile Materials
 - Creep-fatigue Test Methods (ASTM Standard E2760)
- Combining Physics based Models with Service Data for Improved Prognostics

C

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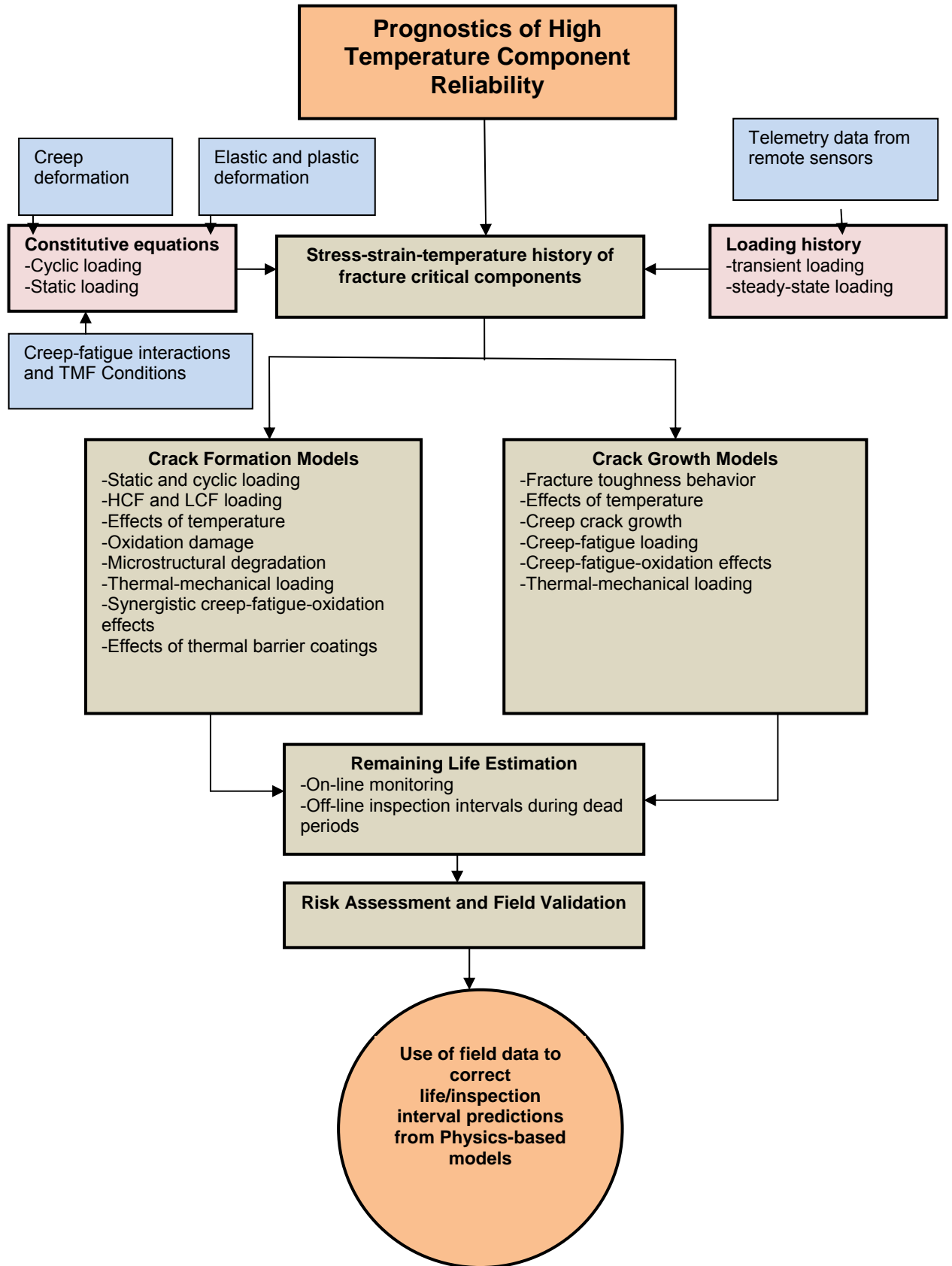


Fig. 1 A methodology for prognostics of high temperature component reliability

Integrity Assessment of H₂ Storage Pressure Vessels

To respond to clean emission requirements from cars and other road vehicles, hydrogen fueled vehicles that utilize fuel cells are predicted to have a strong future demand in big cities around the world. This has created a demand for hydrogen fueling stations where hydrogen can be safely compressed and economically stored at extreme pressures in large pressure vessels. For example, current targets call for storing 35 Kg of H₂ in 750 L capacity tanks. The interior of these vessels are made from ferritic, high strength low alloys steels. It is known that these steels are susceptible to hydrogen embrittlement and cracks, if present, can grow at accelerated rates. This phenomenon is critical in determining the design life of these vessels and also in establishing the safe maximum cyclic stress. Figure 2 from our work shows how crack growth rates in hydrogen vary with the cyclic stress intensity parameter, ΔK compared to in air.

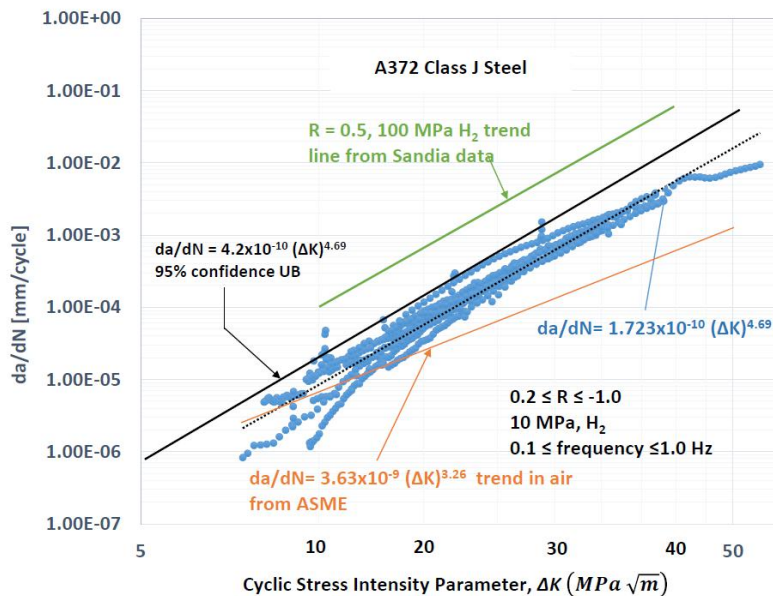


Fig.2 Fatigue crack growth in A372 Grade J steels as a function of ΔK, load ratio, R, and loading frequency clearly showing the accelerated crack growth rate in high pressure H₂.

Our research is focused on understanding the underlying mechanisms of environment assisted cracking in hydrogen and on modeling the effects of loading variables of load ratio and loading frequency and environment severity such as hydrogen pressure. The effort is aimed at identifying conditions for making pressure vessels safe by judiciously choosing the operating conditions and by improving the design of the vessel itself to make it more fracture and fatigue resistant.

Modeling Rupture in Abdominal Aortic Aneurysm

In spite of the advances in medical sciences, cardiovascular diseases remain the leading cause of death. Abdominal aortic aneurysm (AAA) is an irregular expansion of the abdominal aorta due to the weakening of abdominal aortic wall and is considered a form of cardiovascular disease. A patient is said to have AAA when the abdominal aortic diameter increases by 50% of the healthy original diameter. Every year, 500,000 new patients are diagnosed with AAA throughout the world, 150,000 of those in the United States alone. AAA is present in about 2% of elderly (60 years and older), a population group that is rapidly increasing in the developed countries. Abdominal aortic aneurysms are one of the

most lethal aneurysms that can develop in the human body, with a mortality rate approaching 90% in the case of rupture. Every year in the US, a country for which accurate numbers are available, approximately 15,000 to 20,000 people die from AAA, and it is listed as the 13th most common cause of death, and the 10th among men that are 55 years of age and older. Figure 3 shows a finite element model of the formation of aneurysm in a pipe with properties of porcine healthy tissue and one that has suffered degradation of properties due to loss of collagen.

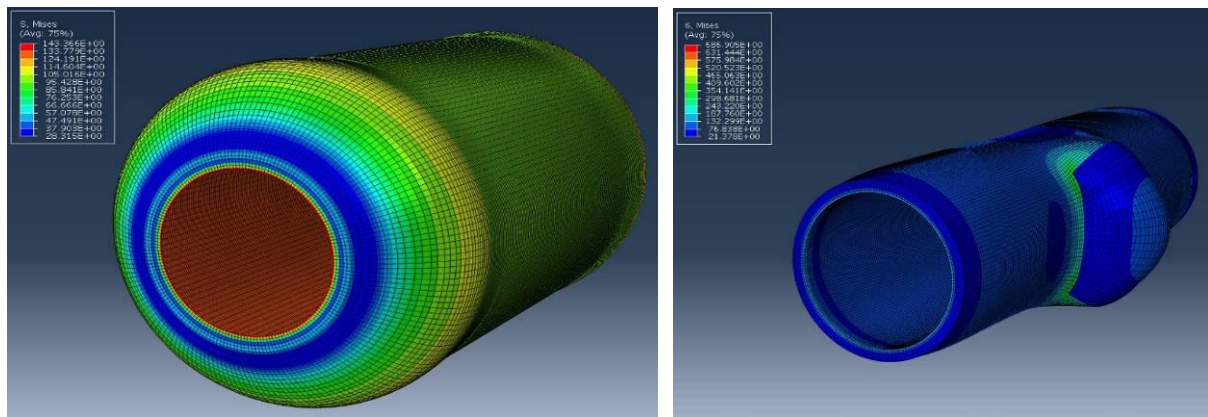


Figure 3 The deformation of a healthy aorta (left) during systole and a collagen degraded aorta (right) during a diastole showing the bulge in the aneurysmal region

Our research focusses on developing constitutive equations for predicting the time-dependent cyclic stress-strain behavior that also account for degradation of properties that occur with aging or with disease progression and using those properties in modeling the progression of AAA. The ultimate goal of this research is to use the model to prevent catastrophic rupture and provide physicians with a prognostic tool that will supplement diagnosis of AAA and save lives. Our understanding of rupture and fracture gained from extensive research in the field for the past six decades can serve as a very useful guide to address this important problem.

Nanoscience and Nanostructures for Solar Cells for Photovoltaics and Solar Fuels

by Arthur Nozik, Member EUAS

Short Biography

Dr. Arthur J. Nozik is a Senior Research Fellow Emeritus at the U.S. DOE National Renewable Energy Laboratory (NREL), Research Professor in the Department of Chemistry and Biochemistry at the University of Colorado, Boulder, and a founding Fellow of the NREL/University of Colorado Renewable and Sustainable Energy Institute (RASEI). In 2009 Nozik was selected as Associate Director of a joint Los Alamos National Lab/NREL Energy Frontier Research Center for DOE, called Center for Advanced Solar Photophysics. Between 2006-2009 he served as the Scientific Director of the Center for Revolutionary Solar Photoconversion under the Colorado Renewable Energy Collaboratory. Nozik received his BChE from Cornell University in 1959 and his PhD in Physical Chemistry from Yale University in 1967. Before joining NREL in 1978, then known as the Solar Energy Research Institute (SERI), he conducted research at the Materials Research Center of the Allied Chemical Corporation (now Honeywell, Inc). Dr. Nozik's research interests include size quantization effects in semiconductor quantum dots and quantum wells, including multiple exciton generation from a single photon; the applications of unique effects in nanostructures to advanced approaches for solar photon conversion to electricity and solar fuels; photogenerated carrier relaxation dynamics in various semiconductor structures; photoelectrochemistry of semiconductor-molecule interfaces; photoelectrochemical energy conversion; photocatalysis; optical, magnetic and electrical properties of solids; and Mössbauer spectroscopy. He has published over 250 papers and book chapters in these fields, written or edited 7 books, holds 11 U.S. patents, and has delivered over 365 invited talks at universities, conferences, and symposia. He has served on numerous scientific review and advisory panels, chaired and organized many international and national conferences, workshops, and symposia, and received several awards in solar energy research, including the 2016 Cross Medal of the Yale Graduate School, 2011 Gustavus Esselen Award from the American Chemical Society, the 2009 Science and Technology Award from the Intergovernmental Renewable Energy Organization associated with the U.N., the 2008 Eni Award from Italy, and the 2002 Research Award of the Electrochemical Society. Dr. Nozik has been a Senior Editor of The Journal of Physical Chemistry from 1993 to 2005 and is on the editorial advisory board of several journals in nanoscience and energy. A Special Festschrift Issue of The Journal of Physical Chemistry honoring Dr. Nozik's scientific career appeared in the December 21, 2006 issue.. Dr. Nozik is a Fellow of the American Physical Society, the American Association for the Advancement of Science; and the Royal Society of Chemistry; he is also a member of the American Chemical Society, the Electrochemical Society, and the Materials Research Society.

Quantum confinement of electronic particles (negative electrons and positive holes) in nanocrystals produces unique optical and electronic properties that have the potential to enhance the power conversion efficiency of solar cells for photovoltaic and solar fuels production at lower cost. These approaches and applications are labeled Future Generation solar photon conversion. Prominent among these unique properties is the efficient formation of more than one electron-hole pair (called excitons in nanocrystals) from a single absorbed photon. In isolated nanocrystals that have 3-dimensional confinement of charge carriers (quantum dots) or 2-dimensional confinement (quantum wires and rods) this process is termed Multiple Exciton Generation (MEG). This manuscript presents a summary of our present understanding of the science of optoelectronic properties of nanocrystals and a prognosis for and review of the technological status of nanocrystals and nanostructures for Future Generation photovoltaic cells and solar cells for liquid and gaseous fuel production.

I. Introduction

Nanostructures of semiconductor materials exhibit quantization effects when the electronic particles of these materials are confined by potential barriers to very small regions of space. The confinement can be in 1 dimension (producing quantum films, also termed quantum wells in the early 1980s as the first examples of quantization in nanoscale materials), in two dimensions (producing quantum wires or rods), or in three dimensions (producing quantum dots (QDs)). Some authors refer to these three regimes as 2D, 1D, or 0D, respectively, although these terms are not as precise. Nanostructures of other classes of materials, such as

metals and organic materials, are also possible, but we will be focused on semiconductor nanostructures and their potential applications for solar energy conversion to solar electricity (photovoltaics) and solar fuels. Semiconductor materials in bulk form currently dominate the field of commercial photovoltaic (PV) power; solar fuels (*direct* conversion of CO₂ and/or H₂O to fuels, such as H₂, alcohols, hydrocarbons, or carbohydrates) are now receiving a high degree of interest and support, but unlike PV, no solar fuels industry exists yet. Biofuels are, of course, derived from solar irradiance driving biological photosynthesis and is a present day industry, but they are not included here in our definition of solar fuels since it is a 2-step process, first involving photosynthesis followed by harvesting and conversion of biomass via dark processes such as fermentation or thermal refining. The nanoscience we discuss here will have relevance mainly for PV, but may also be important for approaches that are being investigated for direct solar fuels production. Nanostructures of crystalline materials are also referred to as nanocrystals; and this term includes a variety of nano-scale shapes with the three types of spatial confinement, including spheres, cubes, rods, wires, tubes, tetrapods, ribbons, cups, discs, and platelets¹. The first six shapes are being intensively studied for renewable energy applications, but the focus here will be on the use of semiconductor QDs plus some discussion of single-walled carbon nanotubes.

II. Status of PV Based on Bulk Semiconductors

PV solar cells operate by absorbing photons from incident solar radiation that have energies above the semiconductor bandgap and thus create negative electrons and positive holes. Bulk inorganic semiconductors have relatively high dielectric constants and at room temperature these photogenerated electronic particles are uncorrelated and move freely in the conduction and valence bands of the semiconductor; they are thus called free (charge) carriers. In organic semiconductors the dielectric constant is low and the photogenerated carriers are correlated and form bound electron-hole pairs that are called excitons. In the former case an internal electric field is required to efficiently separate the free electrons and holes so that they can be collected at oppositely charged electrodes and utilized in a PV cell. This electric field is most commonly produced by a p-n junction in the device; however Schottky junctions between a semiconductor and metal or liquid contacts with appropriate work function differences relative to the semiconductor material can also be used. In organic semiconductors the excitons must be dissociated so that free carriers are formed, separated, and collected at the oppositely charged electrodes. This is usually achieved through a heterojunction having a sufficient band-offset that can drive electrons and holes apart. One ubiquitous feature of all present solar cells is that photons having energies greater than the semiconductor bandgap create free carriers or excitons that have energies in excess of the bandgap; these carriers or excitons are called “hot carriers” or “hot excitons”. This excess electron energy is kinetic free energy and is lost quickly (ps to sub-ps time scales) through electron-phonon scattering, converting the excess kinetic energy into heat. The free carriers or excitons then occupy the lowest energy levels (the bottom and top of the conduction and valence bands, respectively) where they can be removed to do electrical work or lost through radiative or non-radiative recombination. In 1961 Shockley and Queisser² (S-Q) calculated the maximum possible thermodynamic efficiency of converting solar irradiance into electrical free energy in a PV cell assuming: (1) complete carrier cooling, and (2) that the only other free energy loss mechanism was radiative recombination. This detailed balance calculation in the radiative limit yields a maximum thermodynamic efficiency of 31-33% with optimum bandgaps between about 1.1 to 1.4 eV (the bandgaps of Si and GaAs are close to these optimum values). One way used presently to reduce the energy loss due to carrier cooling is to stack a series of semiconductors with different bandgaps in tandem with the largest bandgap irradiated first followed by decreasing bandgaps. In the limit of a large number of different multiple bandgaps matched to the solar spectrum the conversion efficiency can reach 67% at one-sun intensity. Detailed Balance calculations show that with 2 bandgaps the maximum efficiency is 43%, with 3 its 48%, with 4 its 52%, and with 5 its 55%. The present record efficiency in the laboratory of a multijunction solar cell based on 3 junctions (GaInP₂/GaAs/Ge (or GaInAs)) is 41% (under solar concentrations of 140 to 240 suns)³. The highest present one-sun efficiency of single PV junction Si cells in the laboratory is 25%³; the efficiency of commercial PV modules is about 75% of the maximum values measured in the laboratory

III. Solar Cells Utilizing Hot Carriers for Enhanced Conversion Efficiency

In 1982 thermodynamic calculations⁴ first showed that the same high conversion efficiency of a tandem stack of different bandgaps can be obtained by utilizing the excess energy of hot photogenerated carriers before they cooled to the lattice temperature through electron-phonon scattering; in the limit of a carrier temperature of 3000K the conversion efficiency reaches 67%. One way to do this is to transport the hot carriers to carrier-collecting contacts with appropriate work functions (either into an electrolyte redox system in a photoelectrochemical fuel producing cell^{5,6} or a solid state ohmic contact in a PV cell), before the carriers cool. These cells are called hot carrier solar cells⁵⁻⁸. A second approach is to use the excess kinetic

energy of the hot carriers to produce additional electron-hole pairs. In bulk semiconductors this process is called impact ionization⁹ and is an inverse Auger type of process. However, impact ionization (I.I.) cannot contribute to improved quantum yields in present solar cells based on bulk Si, CdTe, CuIn_xGa_{1-x}Se₂, or III-V semiconductors because the maximum QY for I.I. does not produce extra carriers until photon energies reach the ultraviolet region of the spectrum. In bulk semiconductors, the threshold photon energy for I.I. exceeds that required for energy conservation alone because crystal momentum (**k**) must also be conserved⁹. Additionally, the rate of I.I. must compete with the rate of energy relaxation by phonon emission through electron-phonon scattering. It has been shown that the rate of I.I. becomes competitive with phonon scattering rates only when the kinetic energy of the electron is many multiples of the bandgap energy (E_g)¹⁰⁻¹². In bulk semiconductors, the observed transition between inefficient and efficient I.I. occurs slowly; for example, in Si the I.I. efficiency was found to be only 5% (*i.e.* total quantum yield = 105%) at $h\nu \approx 4$ eV ($3.6E_g$), and 25% at $h\nu \approx 4.8$ eV ($4.4E_g$).^{9,13}

IV. Quantum Dots, Multiple Exciton Generation, and Future Generation Solar Cells

Because of spatial confinement of electrons and holes in quantum dots: (1) the e^-h^+ pairs are correlated and thus exist as excitons rather than free carriers, (2) the rate of hot electron and hole (*ie*, exciton) cooling can be slowed because of the formation of discrete electronic states¹, (3) momentum is not a good quantum number and thus the need to conserve crystal momentum is relaxed¹, and (4) Auger processes are greatly enhanced because of increased e^-h^+ Coulomb interaction.¹⁴⁻¹⁷ Because of these factors it has been predicted¹⁴⁻¹⁷ that the production of multiple e^-h^+ pairs will be enhanced in QDs compared to bulk semiconductors; both the threshold energy ($h\nu_{th}$) for electron hole pair multiplication (EHPM) and its efficiency, η_{EHPM} (defined as the number of excitons produced per additional bandgap of energy above the EHPM threshold energy) are expected to be greatly enhanced. In QDs we label the formation of multiple excitons *Multiple Exciton Generation* (MEG)¹⁷; free carriers can only form upon dissociation of the excitons, for example in various PV device structures. The possibility of enhanced MEG in QDs was first proposed in the period 2001-2002^{14,15} and the original concept is shown in Fig.1. Fig 2 presents S-Q detailed balance calculations in the radiative limit for conventional solar cells compared to QD solar cells exhibiting various MEG characteristics regarding the threshold photon energy $h\nu_{th}$ and η_{EHPM} .¹⁸ It has been shown¹⁸ that the threshold photon energy for MEG to occur and its efficiency (defined as the additional photon energy in bandgap units required to create an additional e^-h^+ pairs) are related by the expression:

$$h\nu_{th}/E_g = 1 + 1/\eta_{EHPM} \quad (1)$$

This paper¹⁸ also presents a rigorous derivation of why the appropriate parameter to use when comparing the efficiency of MEG in QDs vs impact ionization in bulk materials is $h\nu/E_g$ and not just the absolute photon energy $h\nu$. When $h\nu/E_g$ is used, the slope of plots of MEG QY vs $h\nu/E_g$ is the MEG efficiency, η_{EHPM} .¹⁸ The use of just $h\nu$ was proposed in a prior publication¹⁹ and led to the invalid conclusion that there is no efficiency difference between MEG in QDs and I.I. in bulk semiconductors. Multiexcitons have been detected using several spectroscopic measurements which are consistent with each other. The first method used was to monitor the signature of multiple exciton generation using transient (pump-probe) absorption (TA) spectroscopy²⁰. The multiple exciton analysis relies on time-resolved TA data taken as a function of the photon excitation (pump) energy. In one type of TA experiment, the probe pulse monitors the interband bleach dynamics with excitation across the QD bandgap^{17,20}; whereas in a second type of experiment the probe pulse is in the mid-IR and monitors the intraband transitions (*e.g.* $1S_e-1P_e$) of the newly created excitons.²⁰⁻²³ In the former case, the peak magnitude of the initial early time (3 ps) photoinduced absorption change created by the pump pulse together with the faster Auger decay dynamics of the generated multiexcitons and the resultant TA signal after the extra excitons have decayed (> 300 ps), are related to the number of excitons created. In the latter case, the TA dynamics of the photoinduced mid-IR intraband absorption after the pump pulse is monitored and analyzed. In refs 20, 21 and 25 the transients are detected by probing either with a probe pulse exciting across the QD bandgap, or with a mid-IR probe pulse that monitors the first $1S_e-1S_p$ intraband transition; both experiments yield the same MEG QYs. The first experimental report of exciton multiplication that was presented by Schaller and Klimov²⁰ for PbSe NCs reported an excitation energy threshold for the efficient formation of two excitons per photon at $3E_g$. But subsequent work has reported that the threshold energy for MEG in PbSe QDs is $2E_g$ ¹⁷ and it was shown that efficient MEG occurs also in PbS¹⁷ and in PbTe QDs²⁴. Additional experiments observing MEG have now been reported for PbSe^{25,26}, CdSe^{27,28}, PbTe²⁴, InAs²⁹, Si³⁰, InP³¹, CdTe³² and CdSe/CdTe core-shell QDs³³. For InP QDs the MEG threshold was $2.1E_g$ and photocharging was shown not to be present in the QD samples³¹. For the CdSe/CdTe QDs time-resolved photoluminescence (TRPL) was used to monitor the effects of multiexcitons on the PL decay dynamics to determine the MEG QY. The time scale for MEG has been reported to be < 100 fs.¹⁷ This ultrafast MEG rate is much faster than the hot exciton cooling rate produced by electron-phonon interactions, and MEG can therefore beat exciton cooling and become efficient.

It is noted that in addition to many reported MEG effects in semiconductor QDs, MEG has also been recently reported in single wall carbon nanotubes^{34,35}. Theoretical considerations³⁶ suggest that MEG should be enhanced in nanotubes compared to QDs. This has been attributed in part to stronger coulomb interactions and the absence of surface states, in nanotubes. Further research is underway on this new and interesting direction for exciton multiplication in various nanostructures other than spherical semiconductor QDS, and in general advances in theory and additional experiments to better understand MEG in various nanostructures are expected.

V. Configurations of QD Solar Cells and Singlet Fission

The two fundamental pathways for enhancing the conversion efficiency (increased photovoltage^{4,37} or increased photocurrent^{38,39}) can be accessed, in principle, in three different QD solar cell configurations; these configurations are shown in Fig. 3 and they are described below. However, it is emphasized that these potential high efficiency configurations are theoretical and to date there is only very limited experimental evidence that hot electron effects can increase the photovoltage of a PV cell⁴⁰. No actual enhanced power conversion efficiencies over present PV solar cells have yet been reported. Notwithstanding, the potential payoff of success in highly efficient MEG in QD-based solar cells justifies continued research in this area. In addition to enhanced efficiency in PV cells, QDs, NCS, and exciton and/or carrier multiplication in semiconductor photoelectrodes could also enhance the efficiency of solar cells for solar fuels production. In this application, MEG effects in semiconductors can be implemented in photoelectrodes for more efficient direct water splitting cells⁴¹, and QDs or NCs of different sizes and shapes can be used in two-junction tandem cells for highly efficient H₂O splitting to H₂ and CO₂ reduction by H₂O to make liquid and gaseous fuels like alcohols and hydrocarbons^{41,42}. A molecular analog of MEG in molecules is singlet fission (SF), whereby an excited singlet state of a molecular chromophore that has its lowest triplet state energy level about half way between the ground state singlet and first excited singlet, produces two triplets from the excited singlet state. Such chromophores can be used in various novel solar cell devices that could exhibit enhanced efficiency in cells for both PV and solar fuels production⁴¹⁻⁴⁷.

1. Photoelectrodes composed of quantum dot arrays

In this configuration (Fig. 3 bottom right), the QDs are formed into an ordered 3-D array with inter-QD spacing sufficiently small such that strong electronic coupling occurs to allow long-range electron transport. If the QDs have the same size and are aligned then this system is a 3-D analog to a 1-D superlattice and the miniband structures formed therein.⁴⁸ The moderately delocalized but still quantized 3-D states could be expected to produce MEG. Also, the slower carrier cooling and delocalized electrons could permit the transport and collection of hot carriers to produce a higher photopotential in a PV or photoelectrochemical cell. Significant progress has been made in forming 3-D arrays of both colloidal and epitaxial IV-VI, II-VI and III-V QDs^{49,50}. The former two systems have been formed via evaporation, crystallization, or self-assembly of colloidal QD solutions containing a reasonably uniform QD size distribution. Although the process can lead to close-packed QD films, they exhibit a significant degree of disorder. Concerning the III-V materials, arrays of epitaxial QDs have been formed by successive epitaxial deposition of epitaxial QD layers; after the first layer of epitaxial QDs is formed, successive layers tend to form with the QDs in each layer aligned on top of each other.^{50,51} Major issues are the nature of the electronic states as a function of inter-dot distance, array order vs disorder, QD orientation and shape, surface states, surface structure/passivation, and surface chemistry. Transport properties of QD arrays are also of critical importance.

2. Quantum dot-sensitized nanocrystalline TiO₂ solar cells

This configuration (Fig. 3 top right) is a variation of a recent promising new type of photovoltaic cell that is based on dye-sensitization of nanocrystalline TiO₂ layers.⁵²⁻⁵⁴ In this latter PV cell, dye molecules are chemisorbed onto the surface of 10-30 nm-size TiO₂ particles that have been sintered into a highly porous nanocrystalline 10–20 μm TiO₂ film. Upon photoexcitation of the dye molecules, electrons are very efficiently injected from the excited state of the dye into the conduction band of the TiO₂, affecting charge separation and producing a photovoltaic effect. For the QD-sensitized cell, QDs are substituted for the dye molecules; they can be adsorbed from a colloidal QD solution⁵⁵ or produced in-situ.⁵⁶⁻⁵⁹ Successful PV effects in such cells have been reported for several semiconductor QDs including InP, InAs, CdSe, CdS, and PbS.⁵⁵⁻⁵⁹ Possible advantages of QDs over dye molecules are the tunability of optical properties with size and better heterojunction formation with solid hole conductors. Also, as discussed here, a unique potential capability of the QD-sensitized solar cell is the production of quantum yields greater than one by MEG.

3. Quantum dots dispersed in organic semiconductor polymer matrices

Recently, photovoltaic effects have been reported in structures consisting of QDs forming intimate junctions with organic semiconductor polymers. In one configuration, a disordered array of CdSe QDs is formed in a hole-conducting polymer—MEH-PPV {poly[2-methoxy, 5-(2'-ethyl)-hexyloxy-p-phenylenevinylene]}.⁶⁰ Upon photoexcitation of the QDs, the photogenerated holes are injected into the MEH-PPV polymer phase, and are collected via an electrical contact to the polymer phase. The electrons remain in the CdSe QDs and are collected through diffusion and percolation in the nanocrystalline phase to an electrical contact to the QD network. Initial results show relatively low conversion efficiencies,^{60,61} but improvements have been reported with rod-like CdSe QD shapes⁶² embedded in poly(3-hexylthiophene) (the rod-like shape enhances electron transport through the nanocrystalline QD phase) and recently⁶³ with newer polymers (PCDTBT, Konarka) that allow for better electrical properties (3.13%, NREL-certified). In another configuration,⁶⁴ a polycrystalline TiO₂ layer is used as the electron conducting phase, and MEH-PPV is used to conduct the holes; the electron and holes are injected into their respective transport mediums upon photoexcitation of the QDs. A variation of these configurations is to disperse the QDs into a blend of electron and hole-conducting polymers (Fig. 3 bottom left). This scheme is the inverse of light emitting diode structures based on QDs⁶⁵⁻⁶⁹. In the PV cell, each type of carrier-transporting polymer would have a selective electrical contact to remove the respective charge carriers. A critical factor for success is to prevent electron-hole recombination at the interfaces of the two polymer blends; prevention of electron-hole recombination is also critical for the other QD configurations mentioned above. All of these possible configurations for QD solar cells are being investigated in various laboratories. Although reasonably high and reliable MEG efficiencies have now been reported, including photocurrent QYs of 160% at 3.2 Eg from QDs bound to single crystal TiO₂ surfaces at photon energies of 3.2 Eg at 77K⁷⁰, no QD-based PV device has yet shown an enhanced power conversion efficiency due to MEG effects. One issue that may be contributing to the low QYs observed thus far is whether there is efficient collection of the additional photogenerated electron and holes before they undergo multiexcitonic decay by Auger processes; the Auger recombination process of multiexcitons occurs within about 20 -50 ps. Further research is necessary to establish these charge separation dynamics in the various QD solar cell configurations.

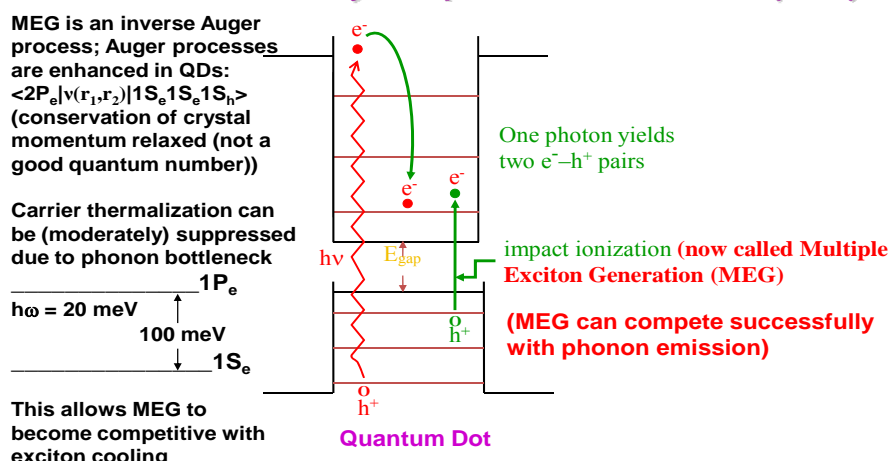
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Figures

Enhanced Photovoltaic Efficiency in Quantum Dot Solar Cells by Multiple Exciton Generation (MEG)



A.J. Nozik, *Ann. Rev. Phys. Chem.* 52, 193, 2001; *Physica E* 14, 115, 2002; in "Next Generation Photovoltaics", Marti & Luque, Eds, AIP, 2003;

Fig. 1 Multiple Exciton Generation in Quantum Dots

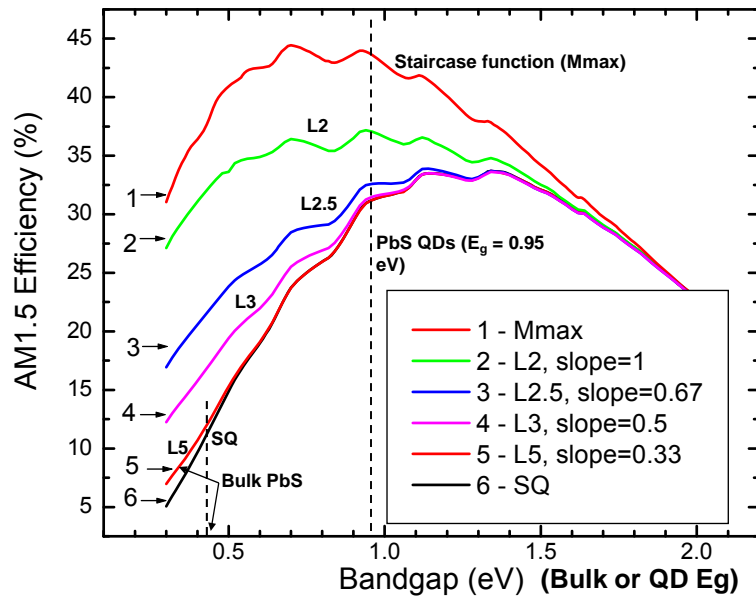


Fig. 2 S-Q calculations for PV power conversion efficiency for various MEG characteristics in QD solar cells compared to PV cells based on bulk semiconductors. L(n) represents the MEG photon energy threshold in units of the number of bandgaps of energy, and the slope value is the MEG efficiency (extra excitons/bandgap of photon energy) beyond the MEG threshold

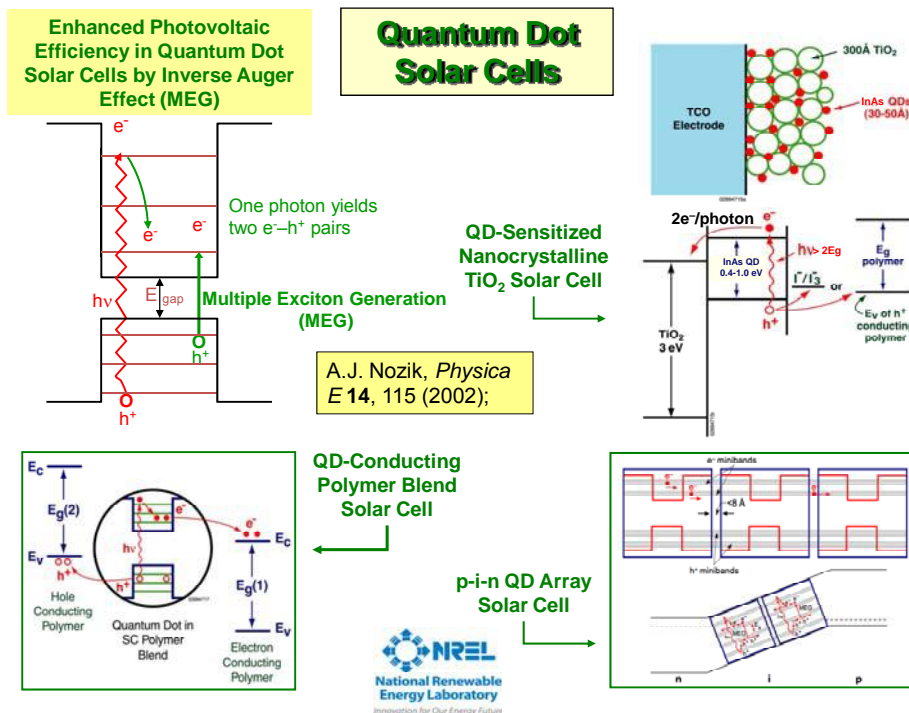


Fig. 3 Generic Quantum Dot PV Solar Cell Configurations

Nanoglasses: A New Kind of Non-crystalline Materials opening the Way to an Age of New Technologies?

by Herbert Gleiter, Member EUAS

Short Biography

Institute of Nanotechnology, Research Center Karlsruhe, Germany

Herbert Gleiter received his Ph.D. in Physics from the University of Stuttgart, Germany. In 1973, Gleiter became Chair Professor of Materials Science at the University of the Saarland in Germany. In 1994, he was appointed Member of the Executive Board of the Research Center Karlsruhe, Germany, and 4 years later he became the Founding Director of the Center's Institute of Nanotechnology. In 2012 the University of Nanjing of Science and Technology founded the "Herbert Gleiter Institute of Nanoscience" and appointed him as the Institute's Founding Director as well as Zijin Professor of this University.

Among Gleiter's more than 40 awards and honors are the Masing Prize of the German Society for Metals (1972); the Leibniz Prize of the German National Science Foundation (1988); Max-Planck Research Prize (1993); Gold Medal of the Federation of European Material Societies (1995); Heyn Medal of the German Society for Materials Science (1998); Heisenberg Medal (1998) and Humboldt Medal (2006); Gold Medal of Acta Materialia (2007); the Von Hippel Award of MRS (2008); the Mehl Award of the TMS Society (2009), the 2009 Blaise Pascal Medal of the European Academy of Sciences and the Cothenius Medal, the highest award of the German National Academy. His publications have been cited more than 22 000 times. Six universities in Europe and abroad awarded him honorary doctorates.

He is a Member of 10 Academies of Science and/or Engineering: e.g. of the German National Academy of Sciences Leopoldina (1999), US National Academy of Engineering (2004), Indian National Academy of Engineering (2006), the American Academy of Arts and Sciences (2004), the Indian National Academy of Sciences (2009), the European Academy of Sciences (2009), the European Academy of Sciences and Arts (2014) as well as the Academia Europaea and the EU Academy of Sciences (2015).

Nano-glasses are a new class of non-crystalline materials. They consist of nanometer-sized clusters that are connected by non-crystalline regions with a new atomic arrangement that was discovered in nano-glasses. By varying the sizes and/or the chemical compositions of the glassy clusters, non-crystalline materials with a similar variety of structures and properties can be generated that are available today in the various crystalline materials which provide the basis for today's technologies. Hence, the technological application of nano-glasses may open the way to a world of new technologies (a "glass age") based on the use different nano-glasses.

The majority of materials that have been utilized by mankind since the Neolithic age are crystalline materials. The oldest known examples are granite and quartz used for producing stone-age tools. More recent examples are light weight metals (e.g. Al), semiconductors (e.g. Si), materials with high strength (e.g. steels), superconductors, ferroelectrics nano-crystalline materials or advanced ferromagnetic materials. The main reason for the preference of crystalline materials is the fact that their properties may be controlled by modifying their defect structure (e.g. by modifying the density of inter-crystalline interfaces) and/or their chemical compositions [1].

Glassy materials, although known for more than 15000 years (e. g. in the form of obsidian), have not been utilized so far in a comparable large variety of technologies. The

most important applications seem to be windows, lenses, optical fibers, amorphous magnets and surface coatings. The main reason for this less frequent use of glasses is that today's glasses are produced most frequently by quenching the melt. Hence, the atomic structures of the resulting glasses are essentially the structures of the molten state at the glass transition temperature.

This production process does not permit to introduce into glasses defects that are, for example, similar to the inter-crystalline boundaries of crystalline materials. As a consequence, one cannot control the properties of the glasses we have today by the controlled modification of their defect and/or chemical microstructures as in crystalline materials.

On the other hand, history of mankind teaches us that it was the controlled modification of the defect and/or chemical microstructures of materials (e.g. by plastic deformation or by alloying) that has opened in the past the way to new ages of technology e.g. the bronze age or the iron age. Hence, the door to a world of new technologies (beyond today's technologies based predominantly on crystalline materials) may be opened if one succeeds in synthesizing non-crystalline materials with controllable modifications of their defect and/or chemical microstructures.

Structural Concept of Nano-glasses

A first promising attempt to open this door are nano-glasses. Nano-glasses are non-crystalline materials with controllable modifications of their defect and/or chemical microstructures. In fact, it is the idea of nano-glasses (Fig. 1) to introduce a high density of glass-glass interfaces by consolidating nanometer-sized glassy clusters (Fig. 1c) with identical or different (Fig. 1d) chemical compositions.

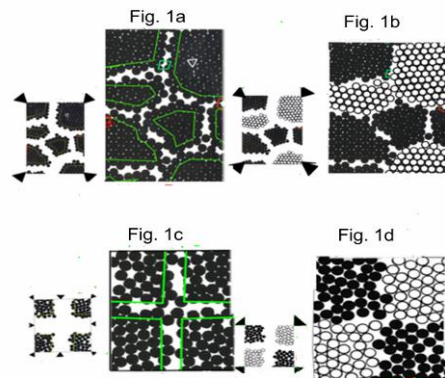


Fig. 1 Analogy between the defect and the chemical microstructure of crystalline materials (upper row of the figure) and of nano-glasses (lower row of the figure). The defect microstructure (Fig. 1a) and the chemical microstructure of a nanocrystalline material (Fig. 1b) are compared in Fig. 1c and in Fig. 1d with the corresponding defect microstructure and the corresponding chemical microstructure of a nano-glass [1].

Fig. 1 displays the analogy between the defect and the chemical microstructure of crystalline materials (upper row of the figure) and of nano-glasses (lower row of the figure). The defect microstructure (Fig. 1a) and the chemical microstructure of a nanocrystalline material (Fig. 1b) are compared in Fig. 1c and in Fig. 1d with the corresponding defect microstructure and the corresponding chemical microstructure of nano-glasses [1]. As may be seen, nano-glasses are structurally analog to the crystalline materials available today that provide the basis for most of today's technologies.

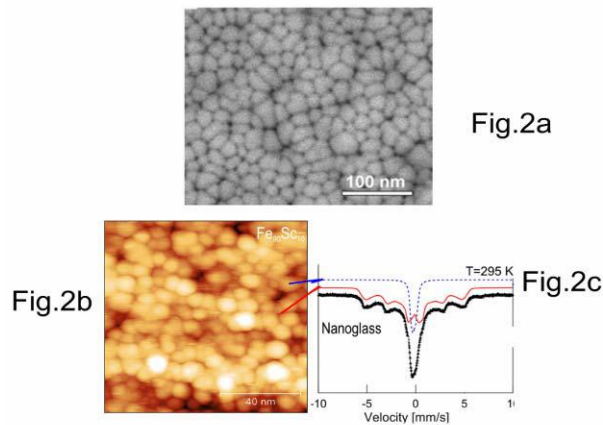


Fig. 2 Electron micrograph (Fig. 2a) and an atomic force micrograph (Fig. 2b) of an $Au_{52}Ag_5Pd_2Cu_{25}Si_{10}Al_6$ nano-glass and Moessbauer spectrum of a $Fe_{90}Sc_{10}$ nano-glass, respectively. As may be seen (Figs. 2a and 2b) the microstructure of the nano-glass consist of nanometer-sized glassy regions connected by interfaces similar to the structure shown in Fig. 1c

Fig 2 displays an electron micrograph (Fig. 2a) and an atomic force micrograph (Fig. 2b) of an $Au_{52}Ag_5Pd_2Cu_{25}Si_{10}Al_6$ nanoglass and of a $Fe_{90}Sc_{10}$ nano-glass, respectively. As may be seen, their microscopic structures consist of nanometer-sized glassy regions connected by interfaces similar to the structure shown in Fig. 1a. The results of studies of the structures of nano-glasses by means of transmission electron microscopy, positron annihilation spectroscopy, wide and small angle X-ray diffraction, elemental mapping, scanning tunnel electron as well as atomic force microscopy, Moessbauer spectroscopy and molecular dynamics (for a review of these studies we refer to ref. [1]) have indicated that the glassy regions and the interfacial regions of a nano-glass differ as far as their atomic and as far as their electronic structures are concerned. The different atomic and electronic structures of the glassy regions and the interfacial regions of a nano-glass (with the same chemical compositions) are - for example - evidenced by different Moessbauer spectra. Fig. 2c displays the different Moessbauer spectra of the glassy regions (a single line spectrum indicated by a blue line) and the interfacial regions (a spectrum consisting of six lines, red curve) of a $Fe_{90}Sc_{10}$ nano-glass indicating that the glassy regions are paramagnetic whereas the interfaces are ferromagnetic at 295K. Similar differences were noted by all the other methods mentioned above [1].

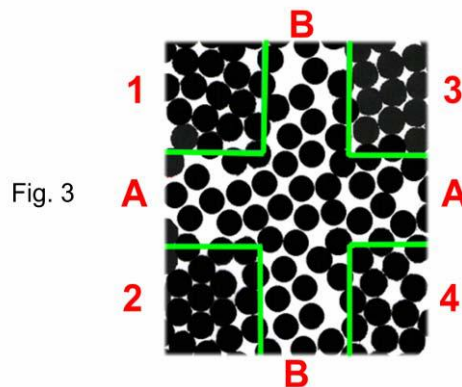


Fig. 3 Structural model of the nano-glass after a relaxation process of 80 ps relaxation time at 300 K and under an external hydrostatic pressure of ~ 5 GPa assuming a Ge interaction potential between the atoms of the nano-glass [1]. As may be seen, the relaxation process resulted in a nano-glass structure consisting of four glassy regions (1, 2, 3 and 4 in Fig. 3) and two interfaces AA and BB.

The structural model of a nano-glass that was deduced from all of these studies [1] is

displayed in Fig. 3. In fact, the nano-glass consists of the regions (1,2,3,4 in Fig 3) with the structure of a glass produced by quenching the melt and the interfacial regions connecting them (AA and BB in Fig 3) with an atomic and electronic structure that has not been known before. The formation of the new non-crystalline and new electronic structures in the interfaces of nano-glasses may be understood [1] in terms of the relaxation of the interfacial atoms of the glassy clusters from their initial sites i.e. from the sites before these clusters were joined together to produce a nano-glass. (For further details we refer to ref. [1]).

New Properties of Nano-glasses

The new non-crystalline atomic structures as well as the new electronic structures of the interfacial regions of nano-glasses were observed to result in new properties (For a summary we refer to ref [1]). For example $\text{Fe}_{90}\text{Sc}_{10}$ nano-glasses were observed to be ferromagnetic at 300 K (Fig. 2c) whereas the corresponding ribbons exhibited paramagnetic properties. By using micro-compression experiments the deformation behavior of a melt-quenched ribbon of a $\text{Sc}_{75}\text{Fe}_{25}$ metallic glass and of a $\text{Sc}_{75}\text{Fe}_{25}$ nano-glass were studied (Fig. 4).

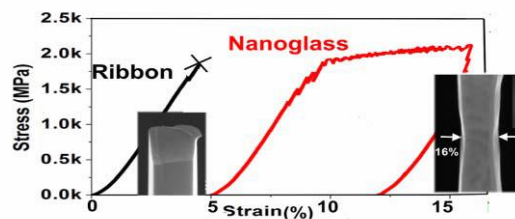


Fig. 4

Fig.4 Stress strain curve of 2 μm pillars of a $\text{Sc}_{75}\text{Fe}_{25}$ nano-glass and of a melt-spun ribbon with the same chemical composition [1]. The inserts show the brittle fracture of the ribbon and the plastic deformation of the nano glass.

The $\text{Sc}_{75}\text{Fe}_{25}$ nano-glass was found to yield at a stress of about 1250 MPa and exhibited extensive plastic flow up to about 15%. The fracture stress was about 1950 MPa. The corresponding glassy ribbons exhibited brittle fracture. $\text{Au}_{52}\text{Ag}_5\text{Pd}_2\text{Cu}_{25}\text{Si}_{10}\text{Al}_6$ nano-glass was noted to exhibit a catalytic activity (Fig.5) for removing silanes by an oxidation process with water that was two orders of magnitude larger than the catalytic activity of the corresponding melt spun ribbon. In a first pioneering study of the biocompatibility of nano-glasses (Fig. 6), layers of $\text{Ti}_{34}\text{Zr}_{14}\text{Cu}_{22}\text{Pd}_{30}$ nano-glass (NGC) were generated [2]. In order to evaluate the cell proliferation on these NGC, about ten thousand osteoblast cells were seeded onto their surfaces. The proliferation of the osteoblasts on the $\text{Ti}_{34}\text{Zr}_{14}\text{Cu}_{22}\text{Pd}_{30}$ nano-glass samples was then compared with the one on the surfaces of pure Ti and the corresponding melt spun ribbons MSR (Fig.6). In a first pioneering study of the biocompatibility of nano-glasses (Fig. 6), layers of $\text{Ti}_{34}\text{Zr}_{14}\text{Cu}_{22}\text{Pd}_{30}$ nano-glass (NGC) were generated [2]. In order to evaluate the cell proliferation on these NGC, about ten thousand osteoblast cells were seeded onto their surfaces. The proliferation of the osteoblasts on the $\text{Ti}_{34}\text{Zr}_{14}\text{Cu}_{22}\text{Pd}_{30}$ nano-glass samples was then compared with the one on the surfaces of pure Ti and the corresponding melt spun ribbons MSR (Fig.6). After 7 days the density of the cells on the NGC surface was 10 to 20-fold higher than the ones on the MSR and on Ti attracting widespread interest in nano-glasses for improved tissue regeneration and the for fast incorporation of implantation in the human body.

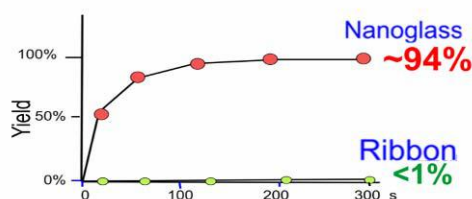


Fig. 5

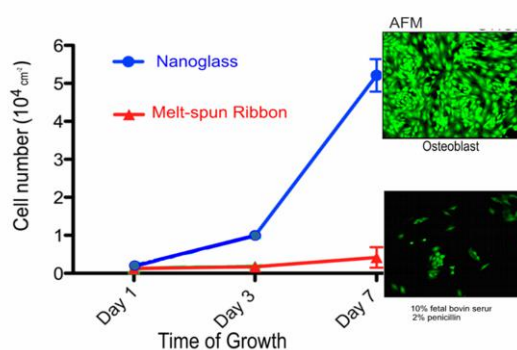
Fig.5 Oxidation of Dimethylphenylsilane at 20°C at 1 atm

Fig. 6

Fig. 6 Cell proliferation at the surface of a melt-spun ribbon and at the surface of a nano-glass with the same chemical composition ($\text{Ti}_{34}\text{Zr}_{14}\text{Cu}_{22}\text{Pd}_{30}$). The micrographs on the right side display the density of the osteoblasts (green color) on the surfaces of both materials after a growth time of 7 days [2].

Historical Outlook

In the past, the understanding and utilization of materials such as metals, semiconductors, ceramics etc. resulted in specific periods of the development of mankind such as the iron age, the bronze age etc. The majority of these materials were crystalline materials because their properties could be controlled by modifying their defect and/or their chemical microstructures.

Today, we seem to be in a comparable situation for materials with non-crystalline structures. In fact, nano-glasses seem to open the way to a new class of non-crystalline materials with controllable defect and/or chemical microstructures resulting in non-crystalline materials with new atomic and new electronic structures and, hence, new properties (in comparison to the properties of the glasses available today that are produced by quenching the melt). Hence, by analogy to the technological developments in the past based on crystalline materials, nano-glasses may permit the development of a large variety of new technologies that are not possible with the glassy materials we have today. In other words, nano-glasses may open the way to a “glass age”.

A prerequisite for a development of this kind is, however, that one succeeds in developing economic methods for producing large quantities of nano-glasses with well controlled microstructures.

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The Effect of Testosterone on Coronary Artery Plaque Volume Assessed by Coronary Computerized Tomographic Angiography: The Cardiovascular Trial of the Testosterone Trials

by Matthew Budoff

Short Biography

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Dr. Budoff has been listed among America's Top Doctors every year since 2005. In the past two years alone, Dr. Budoff has been honored with multiple awards recognizing his professional skills and accomplishments. Of particular note is his receipt of the Einstein Award for Scientific Achievement from the International Biographical Centre, Cambridge, U.K.; being named to the US News list of Top Doctors; and named to "Worlds Most Influential Scientific Minds" in 2014. In 2015, he was named the Endowed Chair of Preventive Cardiology at his institution and was awarded the Arthur S. Agatston Cardiovascular Disease Prevention Award. In 2016, he was awarded the prestigious Gold Medal Award from the Society of Cardiovascular Computed Tomography.

Dr. Budoff works on at least 20 active medical research trials at any given time, and is a frequent lecturer on topics of cardiology at symposia, congresses and annual conferences on every continent. He has authored or co-authored over 864 research papers, seven books, and 45 book chapters.

Importance: Recent studies have yielded conflicting results as to whether or not testosterone treatment increases cardiovascular risk.

Objective: To test the hypothesis that testosterone treatment of older men with low testosterone would retard the progression of noncalcified coronary artery plaque volume.

Design: Double-blinded, placebo-controlled trial

Setting: Nine academic medical centers in the United States

Participants: 170 men ≥ 65 years old with an average of two serum testosterone levels < 275 ng/dL who were enrolled in The Testosterone Trials.

Intervention: Testosterone gel, the dose adjusted to maintain the testosterone level in the normal range for young men, or placebo gel for 12 months.

Main Outcome Measure: Noncalcified coronary artery plaque volume, as determined by coronary computerized tomographic angiography.

Results: At baseline, the participants had a relatively high prevalence of coronary atherosclerosis; 51.5% had a coronary artery calcification score > 300 units. Testosterone treatment was associated with significant increases in noncalcified plaque volume from baseline to 12 months (40 ± 72 mm³) compared with placebo (4 ± 75 mm³) ($p = 0.003$) (primary outcome) and in total plaque volume (57 ± 93 mm³) compared with placebo (21 ± 87 mm³) ($p = 0.006$). Testosterone treatment was associated with a significant increase in

the volume of fibrous plaque (one of the components of noncalcified plaque) ($25 \pm 47 \text{ mm}^3$) compared with placebo ($1.2 \pm 58 \text{ mm}^3$) ($p=0.01$). Testosterone was not associated with a change in coronary artery calcium score (66 ± 154) compared to placebo (113 ± 182) ($p = 0.83$).

Conclusions and Relevance: Testosterone treatment for one year of older men with low testosterone increased noncalcified and total plaque volume, as determined by coronary computerized tomographic arteriography. These increases are concerning, but their clinical importance is uncertain and may depend on the differential effects of testosterone on the individual components of noncalcified plaque. A much larger and longer trial would be needed to determine the risk of testosterone treatment on major cardiovascular adverse events.

Although testosterone replacement is increasingly being used clinically, the cardiovascular benefits and risks of testosterone administration to older men with age-related decline in testosterone levels remain uncertain. Several recent observational studies show a negative association between serum testosterone concentration and adverse cardiovascular outcomes, the metabolic syndrome, diabetes or mortality, associations independent of traditional cardiovascular risk factors.

Studies of the effects of testosterone on cardiovascular clinical outcomes are conflicting. Meta-analyses of clinical trials have shown no association between testosterone treatment and cardiovascular adverse events, but none of the individual trials included were designed to assess these events prospectively. A recent clinical trial in older men with mild mobility impairment showed an excess of cardiovascular adverse events in men treated with testosterone compared with placebo, but another trial in a similar population did not. These trials were also not designed to assess cardiovascular adverse events. Retrospective studies using large databases of the association of cardiovascular adverse events in men who were taking testosterone compared with those who were not also have yielded conflicting results.

The Testosterone Trials (TTrials), a group of seven placebo-controlled, coordinated trials, were designed to determine the efficacy of testosterone treatment of men ≥ 65 years with low testosterone concentrations for no apparent reason other than age. We designed one of the seven trials – The Cardiovascular Trial – to test the hypothesis that testosterone treatment of older men with low testosterone would retard the progression of noncalcified coronary artery plaque volume, assessed by coronary computed tomographic angiography (CCTA), as an indicator of coronary atherosclerosis.

METHODS

Study Design

To qualify for the TTrials overall, a participant had to qualify for at least one of the three main trials (Sexual Function, Physical Function and Vitality). Those who qualified overall could participate in any of the others for which they qualified. Participants were allocated to receive testosterone or placebo gel for one year. This report describes the results of the Cardiovascular Trial.

The TTrials and the Cardiovascular Trial protocols were approved by the institutional review boards of the participating sites. All participants provided written informed consent

before trial-related procedures were conducted. Participant safety and trial conduct were overseen by an Independent Data and Safety Monitoring Board.

Participants

Participants were recruited primarily by mass mailings. Respondents were screened by telephone and then during two clinic visits. The main overall inclusion criteria were men ≥ 65 years, serum testosterone levels that averaged < 275 ng/dL on two morning samples, and subjective complaints and objective evidence of sexual dysfunction, physical dysfunction and/or reduced vitality. The main exclusion criterion was high risk of prostate cancer. We also excluded men who had a history of myocardial infarction or stroke within the previous three months and who had a systolic blood pressure > 160 mm Hg or diastolic blood pressure > 100 mm Hg.

Additional exclusion criteria for the Cardiovascular Trial were related to CCTA, conditions that either increased the risk of performing the procedure (estimated glomerular filtration rate < 60 ml/min/1.73m²) or known allergy to iodinated contrast medium) or made the procedure technically impractical (weight > 300 pounds, inability to hold the breath for 10 seconds, a prior diagnosis of tachycardia or irregular heart rhythm, eg, atrial fibrillation, or coronary artery bypass graft surgery).

Testosterone Treatment

Participants were allocated to treatment by minimization, which assigned them to the optimally-balancing treatment with 80% probability. The balancing variables included participation in the main trials, trial site, age under or over 75 years, screening testosterone under or over 200 ng/dL, and use of antidepressants and PDE-5 inhibitors. There was only one treatment assignment, regardless of the number of trials in which a man participated.

Testosterone was administered as a 1% gel in a pump bottle (AndroGel, AbbVie). Placebo gel was similar. The dose was initially 5g a day and was adjusted, if necessary, on the basis of testosterone levels measured at a central laboratory (Quest Clinical Trials, Valencia CA) at months 1, 2, 3, 6 and 9, to try to keep the serum concentration within the normal range for young men. To maintain blinding when the dose was adjusted in a man taking testosterone, the dose was changed simultaneously in a man taking placebo.

Assessments

The concentration of testosterone was measured on sera drawn at baseline and months 3, 6, 9 and 12 and stored at -80°C . This assay was performed at the Brigham Research Assay Core (Boston MA).

Coronary artery plaque volume was assessed by CCTA at 9 of the 12 TTrial clinical sites. Each of these sites had a ≥ 64 -slice CCTA scanner and a staff experienced in CCTA, as determined by a questionnaire. Pre-contrast scans for evaluation of coronary artery calcium and post-contrast scans for evaluation of coronary artery plaque volume were performed at baseline and 12 months. If a participant who had a baseline scan developed an allergy to contrast medium or experienced a decrease in eGFR to ≤ 60 before the month 12 scan, only the pre-contrast scan was performed at month 12.

All scans were evaluated at a central reading center by an investigator blinded to treatment assignment. Coronary images were transferred to the workstation with the use of

semiautomated plaque analysis software (QAngioCT Research Edition Version 2.0.5, Medis Medical Imaging Systems) and evaluated using a protocol for quantitative plaque assessment. Vessel diameters >1.5 mm were evaluated and assessed based on a Society of Cardiovascular Computed Tomography 17-segment coronary artery model.

The reader, blinded to both treatment arm and date of scan, evaluated the baseline and month 12 scans side by side to ensure like segments were compared and measured. The area of each coronary plaque visualized in at least 2 adjacent slices (reconstructed slice thickness 0.6 mm) was determined on all affected slices. The total plaque per segment was summed over all segments with plaque. In addition, each coronary territory (right coronary artery, left main, left anterior descending and left circumflex artery) was scored according to presence of the most significant lesion.

The volumes of four types of coronary artery plaque – low attenuation, fibro-fatty, fibrous and dense calcium - were calculated by the Hounsfield unit threshold. The Hounsfield unit threshold was changed dynamically by the software, as plaque attenuation values are affected by luminal contrast densities. The sum of the low attenuation, fibro-fatty and fibrous plaque volumes was considered as noncalcified noncalcified plaque volume, which was the primary outcome. The sum of all four was total plaque volume, a secondary outcome. Coronary artery calcium score, a secondary outcome, was determined on pre-contrast scans as previously described

Statistical Analyses

The effects of testosterone on all outcomes were assessed using a multivariate linear model that adjusts for baseline plaque volume and all balancing variables used in the minimization procedure: study site, indicator variables of participation in each primary efficacy trial, baseline testosterone concentration (\leq or >200 ng/dL), age (\leq or > 75), use of anti-depressants, and use of PDE-5 inhibitors as covariables. All participants with a baseline and 12-month plaque volume measurement were included in the analysis. Significance of the treatment effect on plaque volume was assessed using the two-sided Wald test and confidence interval. A sensitivity analysis to assess the potential impact of missing data was performed with a multiple imputation approach in which all known and measured risk factors for cardiovascular disease were used to impute the missing values. No adjustments were made for multiple testing.

The sample size for this trial was based on an observational CT angiography study in older men using techniques similar to those employed in other TTrials. Using a standard deviation of 26 from scans at two time points approximately one year apart in that study, we calculated that we needed 140 men, 70/arm, to have both baseline and 12 month scans to provide 80% power to detect a difference of 12 mm³ in noncalcified plaque volume from baseline to 12 months.

RESULTS

Participants

Of the 460 men enrolled in the TTrials at the nine sites participating in the Cardiovascular Trial since it began enrolling in April 2011 (27 months after the main trials began enrolling), 170 consented and enrolled, and 166 had a baseline scan, 86 in the testosterone arm and 80 in the placebo arm (Figure 1). A total of 138 men had a month 12 scan, 73 in

the testosterone arm and 65 in the placebo arm, that could be analyzed. Nine men in the testosterone arm and 11 men in the placebo arm did not have month 12 scans even though they were still enrolled, either because they developed a reason for exclusion or refused to have the second scan.

At baseline, the participants had relatively high rates of obesity and concomitant illnesses, such as hypertension, hyperlipidemia and diabetes, as well as relatively high 10-year risk of cardiovascular disease by the American College of Cardiology/American Heart Association risk calculator, 24% in the testosterone arm and 27% in the placebo arm. Atherosclerosis assessed radiographically by coronary artery calcification score >300, was also high; 60.3% in the testosterone arm and 43.8% in the placebo arm. Testosterone treatment increased the serum concentrations from unequivocally low to mid-normal for young men by month 3 and maintained that level for through month 12 (Figure 1). Testosterone treatment also increased the levels of free testosterone and estradiol to mid-normal for young men.

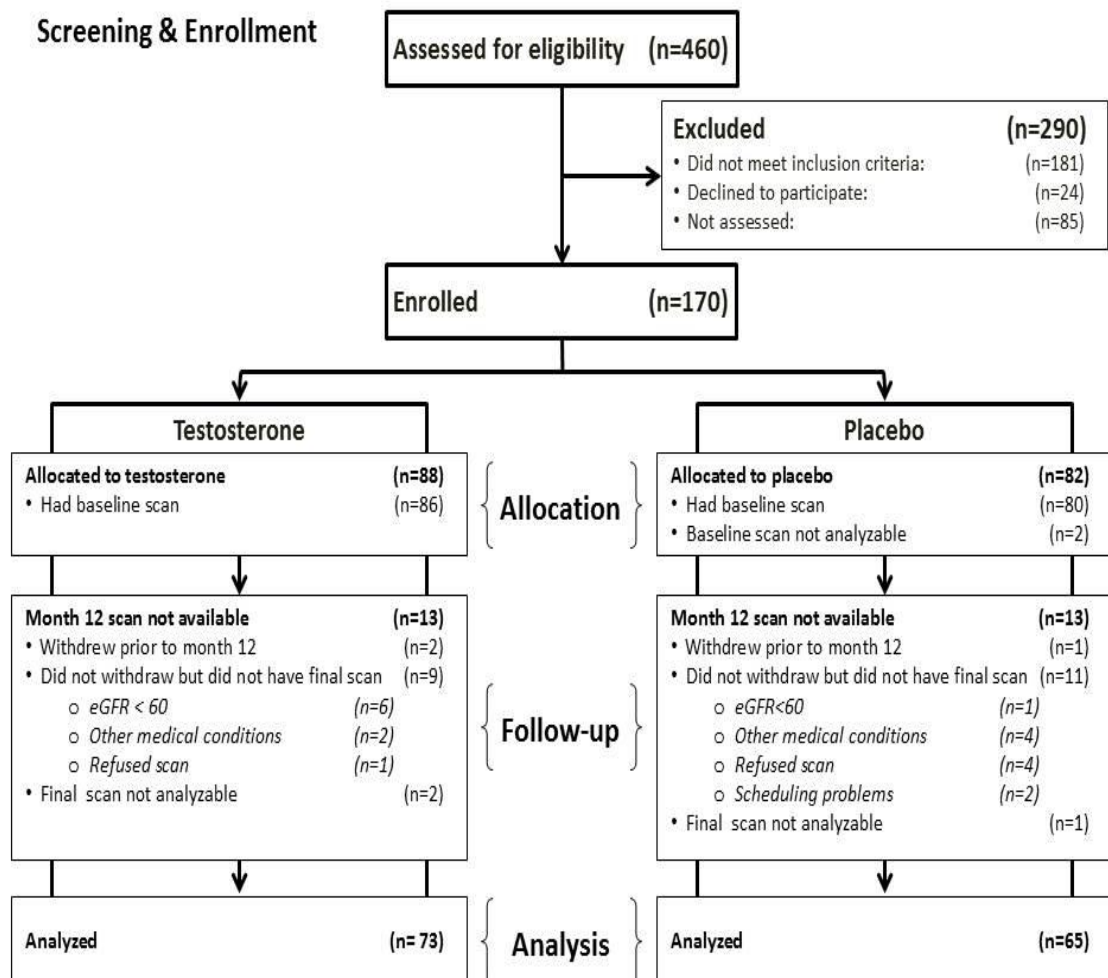


Fig. 1 Screening and retention of participants in the Cardiovascular Trial

Chemiosmosis and the Mechanism of Active Transport

by H. Ronald Kaback, Member EUAS

Short Biography

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Elected Member, EU Academy of Sciences

The lactose permease of *Escherichia coli* (LacY) specifically binds and catalyzes symport of D-galactose and D-galactopyranosides with an H⁺ (galactoside/H⁺ symport), but does not recognize the analogous glucopyranosides, which differ only in the orientation of the C4-OH of the pyranosyl ring (reviewed in 1, 2). Typical of many major facilitator superfamily (MFS) members, LacY couples the free energy released from downhill translocation of H⁺ in response to an H⁺ electrochemical gradient ($\Delta\tilde{\mu}_{H^+}$) to drive accumulation of galactopyranosides against a concentration gradient. Since coupling between sugar and H⁺ translocation is obligatory, in the absence of $\Delta\tilde{\mu}_{H^+}$, LacY can also transduce the energy released from the downhill transport of sugar to drive uphill H⁺ transport with the generation of $\Delta\tilde{\mu}_{H^+}$, the polarity of which depends upon the direction of the sugar gradient. However, the mechanism by which this so-called chemiosmotic process occurs remains obscure. The work described herein aims at clarifying the specific steps underpinning the mechanism of galactoside/H⁺ symport as a paradigm of the MFS.

Structural evidence for an occluded intermediate. Initial x-ray structures of LacY were obtained with a conformationally restricted mutant C154G (3, 4) and WT LacY (5), and they are in an indistinguishable inward (cytoplasmic)-open conformation (**Fig. 1**). At the same time, a similar structure was determined for the glycerol-3-phosphate permease (GlpT) (6), which catalyzes phosphate/glycerol-3-phosphate exchange. The structures consist of two 6-helix bundles related by a quasi two-fold symmetry axis perpendicular to the membrane plane, linked by a long cytoplasmic loop between helices VI and VII. Furthermore, in each 6-helix bundle, there are two 3-helix bundles with inverted symmetry. The two 6-helix bundles surround a deep hydrophilic cavity tightly sealed on the periplasmic face and open to the cytoplasmic side only (an inward-open conformation). The initial structures led to the “rocker-switch” model for transport in which the two 6-helix bundles rotate against each other around the middle of the protein, thereby exposing the substrate-binding site alternatively to either side of the membrane (*aka*, the alternating access model).

Although LacY contains 65-70% unequivocally hydrophobic side chains and crystal structures reflect only a single lowest energy conformation, the entire-backbone appears to be accessible to water (7-9). In addition, an abundance of biochemical and spectroscopic data demonstrates that galactoside binding causes the molecule to open reciprocally on either side of the membrane, thereby providing almost unequivocal evidence for an alternating-access model (see below). The first structure of LacY was obtained with a density at the apex of the central cavity, but because of limited resolution, the identity of the bound sugar and/or side-chain interactions were difficult to specify with certainty. However, biochemical and spectroscopic studies show that LacY contains a single galactoside-binding site and that the residues involved in sugar binding are located at or near the apex of a central, aqueous cavity in the approximate middle of the molecule.

Among the conserved residues in LacY and many other MFS members are two Gly-Gly pairs between the N- and C-terminal 6-helix bundles on the periplasmic side of LacY at the ends of helices II and XI (Gly46 and Gly370, respectively) and helices V and VIII (Gly159 and Gly262, respectively) (10). When Gly46 (helix II) and Gly262 (helix VIII) are replaced with bulky Trp residues (**Fig. 2**), transport activity is abrogated with little or no effect on galactoside affinity, but markedly increased accessibility of galactoside to the binding site is observed indicating that the G46W/G262W mutant is open on the periplasmic side (11). Moreover, site-directed alkylation and stopped-flow binding kinetics indicate that the G46W/G262W mutant is physically open on the periplasmic side (an outward-open conformation).

An X-ray structure of LacY mutant G46W/G262W co-crystallized in the presence of the relatively high-affinity, symmetrical lactose analogue β -D-galactopyranosyl-1-thio- β -D-galactopyranoside (TDG) was determined to 3.5-Å resolution, and importantly, crystals were not obtained in the absence of a galactoside (12). Two molecules in the asymmetric unit are adjacent to one another, but in opposite-facing orientations. Surprisingly, both molecules are in an almost occluded conformation with a narrow periplasmic opening and a single molecule of TDG in the central sugar-binding site.

A space-filling view of the molecule from the periplasmic side (**Fig. 3A**) reveals the bound TDG through an opening that is too narrow to allow entrance or exit of the sugar (~ 3 Å at the narrowest point; **Fig. 3B**) (13). In contrast, the cytoplasmic side of the molecule is tightly sealed (**Fig. 3C**). The double-Trp mutant is sufficiently open to bind galactoside rapidly (11), but when binding occurs and the mutant attempts to transition into an occluded state, it cannot do so completely because the bulky Trp residues block complete closure. Thus, the mutant binds galactoside, which initiates transition into an intermediate occluded state, which it cannot complete, and this accounts for why the mutant is completely unable to catalyze transport of any type across the membrane. It is also apparent that the transport cycle includes an occluded intermediate conformer.

A TDG molecule is clearly defined in the almost occluded central cavity (**Fig. 4**) that allows assignment of likely H-bond interactions with the protein, although interatomic distances are only estimates at 3.5-Å resolution. Specificity is directed towards the galactopyranoside ring, and α -galactosides bind with higher affinity than the β -anomers (14-18). One galactopyranosyl ring of TDG stacks hydrophobically with Trp151 (helix V), confirming biochemical (19) and

spectroscopic (20) findings. Glu269 (helix VIII) is the acceptor of H bonds from the C4-OH and C3-OH groups of the galactopyranosyl ring, indicating that it is probably the primary determinant for specificity. Even conservative replacement with an Asp abolishes binding and inactivates lactose transport (21-23). The η_1 NH₂ of Arg144 (helix V) donates an H bond to O5 in the ring and is also within H-bond distance of the C6-OH. The η_2 NH₂ group of Arg144 donates H bonds to the C2'-OH of TDG and to Glu126 O \square 2. Conservative replacement of Arg144 with Lys, as well as neutral replacements, virtually destroys binding and transport (23, 24). Glu126 (helix IV) acts as an H-bond acceptor from the C2'-OH of TDG and is an H-bond acceptor from the η_2 NH₂ of Arg144. Replacement with Asp causes markedly diminished binding affinity; removal of the carboxyl group abolishes binding and transport (22-24).

Remarkably, His322 (helix X), long thought to be involved in H⁺ transport by implication, likely acts as an H-bond donor/acceptor between the \square NH of the imidazole ring and the C3-OH of TDG, and is stabilized by an H-bond donor/acceptor between the δ \square \square of the imidazole and the OH of Tyr236, which was also thought to be involved in H⁺ transport. All replacements for His322 exhibit little or no binding and no transport activity (23, 25, 26). Finally, Asn272 (helix VIII) donates an H bond to the C4-OH of TDG; Gln is the only replacement tolerated by LacY with respect to binding and transport (27).

In addition to the residues involved in galactoside binding, Cys148 (helix V), well known with respect to substrate protection against alkylation (reviewed in 28), is close to bound TDG, but not sufficiently close to interact directly (**Fig. 5**). Similarly, replacement of Ala122 (helix IV) with bulky side chains, or alkylation of A122C with bulky thiol reagents causes LacY to become specific for the monosaccharide galactose, and disaccharide binding and transport are blocked (29). However Ala122 does not make direct contact with TDG either. Asp240 (helix VII) and Lys 319 (helix X) interact relatively weakly, and mutants with double-neutral replacements (Cys or Ala) exhibit low but significant ability to catalyze lactose accumulation (30-32).

Although Glu325 (helix X) and Arg302 (helix IX) do not make direct contact with bound galactoside, both are critically involved in coupled H⁺ translocation. Neutral replacement of either residue yields mutants that are defective in all transport reactions that involve net H⁺ transport, but catalyze equilibrium exchange and/or counterflow as well or better than WT (1, 2).

Sugar binding involves induced fit. In the structure of single-Cys122 LacY with covalently bound MTS-Gal, a suicide inactivator for this mutant (33), the galactosyl moiety occupies the same position in the protein as in the double-Trp mutant (34). In addition, two important ligands—Trp151 and Glu269—interact with the galactopyranosyl ring (**Fig.6A**). However, as opposed to the almost occluded, open-outward conformation of the double-Trp mutant, LacY with covalently bound MTS-Gal in the binding site exhibits an inward-open conformation (**Fig. 6B**), indicating that the galactoside must be fully liganded in order for LacY to transition into the occluded state. In view of this consideration and observations indicating that the alternating access mechanism of LacY is driven by galactoside binding and dissociation and not by $\Delta\mu_{H^+}$ (1, 2, 35-37), it seems highly likely that sugar binding involves induced fit. By this means, the N- and C-terminal bundles converge as given side chains from both the N- and C-terminal helix bundles ligate the galactoside. The energetic cost of binding and the resultant conformational change is regained upon sugar dissociation and provides the energy for a further structural change that allows deprotonation. With respect to induced- fit, it is also notable that mutation of any single binding-site residue causes a marked decrease or complete loss of affinity (23). In brief, the mechanism of LacY resembles that of an enzyme, the difference being that the protein rather than the substrate forms the transition state.

Seven independent lines of support for the alternating access model. As postulated, alternating access involves reciprocal access of galactoside- and H⁺- binding sites to either side of the membrane. Over the past few years, almost incontrovertible evidence for this structural mechanism has accrued with LacY (reviewed in 38, 39):

1. Since thiol crosslinking yields the closest distance between Cys residues, it was suggested that galactoside binding induces closure of the cytoplasmic cavity (3).
2. Site-directed alkylation of Cys replacements at every position in LacY shows that Cys replacements on the periplasmic side exhibit increased reactivity upon galactoside binding,

- while those on the cytoplasmic side show decreased reactivity (40-45).
3. Single-molecule fluorescence energy transfer (smFRET) studies indicate that the periplasmic side opens and the cytoplasmic cavity closes upon sugar binding (46).
 4. Double electron-electron resonance (DEER) reveals that LacY exists in at least 4 conformations even in the absence of galactoside and that galactoside binding induces a shift in the population towards longer distances on the periplasmic side and shorter distances on the cytoplasmic side (47, 48).
 5. Site-directed thiol cross-linking shows that the periplasmic cavity must open and close for transport to occur. Furthermore, the periplasmic side opens upon galactoside binding to approximately the same extent as observed with DEER (49).
 6. Trp151→*p*-nitrophenyl- α -D-galactopyranoside (NPG) FRET exhibits practically identical kinetics of galactoside binding and displacement with LacY in inward- and outward-facing conformations (50).
 7. Utilization of Trp→bimane or His→Trp FRET to determine opening/closing of periplasmic or cytoplasmic cavities combined with Trp151→NPG FRET to measure galactoside binding, both in real time, shows that opening/closing are reciprocal and that opening of the periplasmic cavity controls closing of the cytoplasmic cavity (12, 51-53).

Mechanism of lactose/H⁺ symport. The affinity of WT LacY for galactosides (K_D) varies with pH to yield an apparent pK^{app} of ~ 10.5 (23, 51, 54). In addition, sugar binding to purified LacY in detergent does not induce a change in ambient pH under conditions where binding or release of 1 H⁺/LacY can be determined (54). Therefore, LacY is protonated over the physiological range of pH (**Fig. 7**). These observations and many others (see 1, 2) provide evidence for a symmetrical ordered kinetic mechanism in which protonation precedes galactoside binding on one side of the membrane, and follows sugar dissociation on the other side. Recent observations (see 55) also suggest that a similar ordered mechanism may be common to other members of the MFS as well. Importantly, as mentioned above, mutants with neutral replacements for Glu325 catalyze equilibrium exchange and counterflow (the shaded reactions in **Fig. 8**), but do not catalyze any reaction involving net H⁺ transport (56, 57). Dramatically, the pH titration observed is abolished in mutant E325A and mutants with other neutral replacements for Glu325, which bind with high affinity up to pH 11 when LacY begins to denature. This behavior is highly unusual and suggests that Glu325 may be the sole residue directly involved in H⁺ binding and transport [all 417 residues in LacY have been mutated and tested for transport activity (22)]. Thus, LacY cannot sustain a negative charge on Glu325 and bind galactoside simultaneously, and Glu325 must be protonated to bind sugar.

In a recent study (58), pH- and substrate-dependent conformational changes were studied in a monolayer of immobilized LacY on a modified gold layer in an attenuated total reflectance (ATR) cell. Surface enhanced IR absorption spectra (SEIRAS) were obtained for WT LacY and mutant E325A, as well as alkali-stable mutants LacY_{ww} and LacY_{ww}/E325A, which allowed identification of Glu325 *in situ* and the direct demonstration that Glu325 has a pK_a of 10.5 ± 0.1 .

But deprotonation is also critical for turnover, and with an apparent pK_a of 10.5, how does deprotonation occur? One possibility is that the pK_a of Glu325, which is in a hydrophobic pocket, may decrease by becoming more accessible to water. However, evidence has been presented indicating that Arg302 is important in this capacity (59, 60). Like neutral replacements for Glu325, mutants R302A and R302S are also specifically defective in translocation reactions that involve H⁺ translocation--accumulation of lactose against a concentration gradient, as well as efflux—but they bind ligand and catalyze equilibrium exchange. Perhaps the positively charged guanidinium group at position 302 facilitates deprotonation of Glu325. Although Tyr236 lies between Arg302 and Glu325 in the current structure (**Fig. 5**), double-mutant R302C/E325C exhibits excimer fluorescence when labeled with pyrene maleimide (61) and double-mutant R302H/E325H binds Mn(II) with μM affinity (62). Therefore, Arg302 and Glu325 may assume closer proximity in another conformation of LacY. Interestingly, a similar mechanism has been suggested for H⁺ transport through the F_o portion of F₁/F_o-ATPase where an Arg residue in subunit *a* is postulated to facilitate deprotonation of an Asp residue in the *c* subunit (reviewed in 63, 64).

Since equilibrium exchange and counterflow do not involve $\Delta\mu_{H^+}$, it is apparent that the

conformational change resulting in alternating accessibility of galactoside- and H⁺-binding sites to either side of the membrane is the result of sugar binding and dissociation, and not $\Delta\tilde{\mu}_{H^+}$ (reviewed in 1, 2). Moreover, lactose/H⁺ symport from a high to a low lactose concentration in the absence of $\Delta\tilde{\mu}_{H^+}$ exhibits a primary deuterium isotope effect that is not observed for $\Delta\tilde{\mu}_{H^+}$ -driven lactose/H⁺ symport, equilibrium exchange or counterflow (65, 66). Thus, it is likely that the rate-limiting step for lactose/H⁺ symport in the absence of $\Delta\tilde{\mu}_{H^+}$ is deprotonation (also see 67, 68), while in the presence of $\Delta\tilde{\mu}_{H^+}$, opening of apo LacY on the other side of the membrane is rate limiting. In other words, by changing the rate-limiting step, $\Delta\tilde{\mu}_{H^+}$ causes more rapid cycling.

A mechanism for chemiosmotic lactose/H⁺ symport. Taken as a whole, the observations suggest the following considerations regarding the mechanism of chemiosmotic coupling in LacY: (i) Symport in the absence or presence of $\Delta\tilde{\mu}_{H^+}$ is the same overall reaction. The limiting step for lactose/H⁺ symport in the absence of $\Delta\tilde{\mu}_{H^+}$ is deprotonation (a kinetic isotope effect is observed with D₂O). The limiting step in the presence of a $\Delta\tilde{\mu}_{H^+}$ is likely the conformational change associated with opening of the cavity on the other side of the membrane. (ii) LacY must be protonated (possibly Glu325 specifically) to bind sugar (the pK_a for binding is ~10.5 and abolished in mutants with neutral replacements for Glu325). (iii) Sugar binding and dissociation--not $\Delta\tilde{\mu}_{H^+}$ --are the driving force for alternating access. (iv) Sugar binding involves induced fit causing transition to an occluded intermediate that undergoes alternating access. (v) Sugar dissociates, releasing the energy of binding. (vi) A conformational change allows Arg302 to approximate protonated Glu325, resulting in deprotonation. (vii) Apo LacY opens on the other side of the membrane, and the cycle is reinitiated.

Strikingly, accumulation of galactoside against a concentration gradient does not involve a change in K_D on either side of the membrane, but the pK (the affinity for H⁺) decreases markedly. Moreover, it is apparent that $\Delta\tilde{\mu}_{H^+}$ does not have a direct effect on the global structural change that corresponds to alternating access. Thus, transport is driven chemiosmotically, and $\Delta\tilde{\mu}_{H^+}$ acts kinetically to control the rate of the process.

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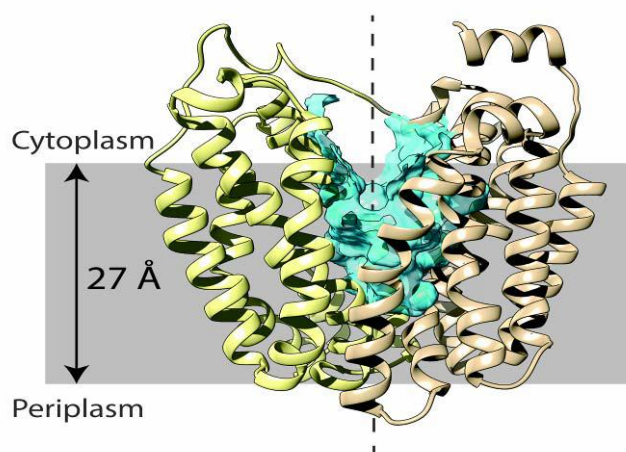


Figure 1: LacY ribbon presentation in an inward-open conformation with a 2-fold axis of symmetry (broken line). Left, N-terminal helix bundle, light yellow; right, C-terminal helix bundle, tan. Cytoplasmic side at top. Blue region, hydrophilic cavity. Gray shaded area, membrane.

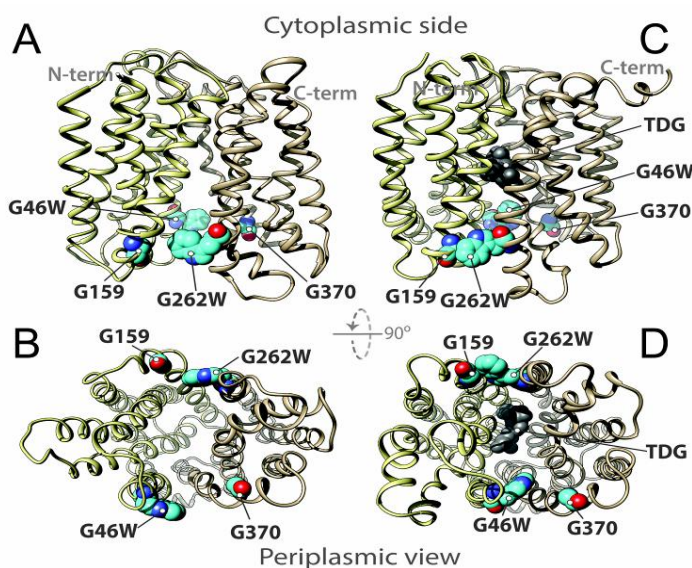


Figure 2: Trp replacements in two pairs of Gly–Gly residues that connect the N- and C-terminal six-helix domains on the periplasmic side of LacY. The 12 transmembrane helices that make up LacY are light yellow (N-terminal bundle) and tan (C-terminal bundle). Gly residues 159 and 370 in helices V and XI, respectively, and Trp replacements G46W (helix II) and G262W (helix VIII) are indicated. The putative outward-open structure is viewed from the side (A) or from the periplasm (B). The crystal structure of the almost occluded, narrow outward-open conformer of LacY with Gly→Trp replacements at positions 46 and 262 and bound galactoside (dark gray) are viewed from the side (C) or the periplasm (D), respectively.

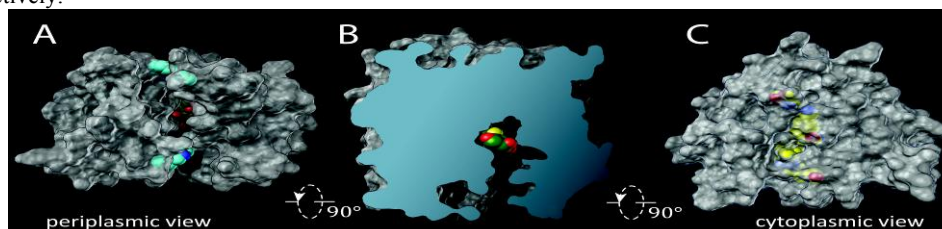


Figure 3: Surface renditions of LacY G46W/G262W molecule A. (A) View from the periplasmic side showing TDG (green and red spheres) just visible within the molecule; Trp residues shown in blue. (B) Slab view. (C) View from the cytoplasmic side with the residues that form a zipper-like motif to seal that side.

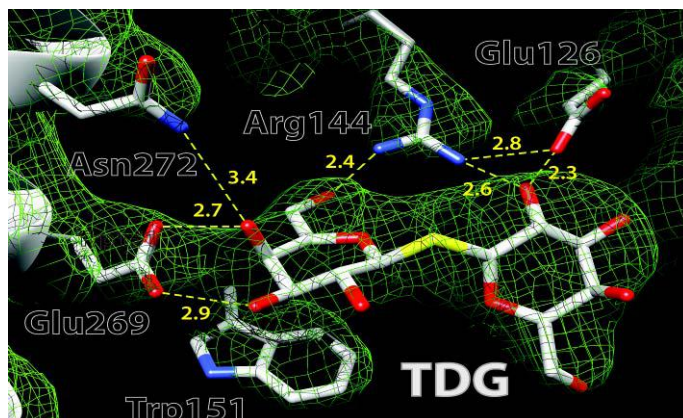


Figure 4: Electron density map contoured at 1σ (green mesh) of the sugar-binding site of LacY G46W/G262W. The density is superimposed on the structure, which is shown as sticks, with carbon atoms in gold, oxygen atoms in red, and nitrogen atoms in blue. Broken lines represent putative H bonds.

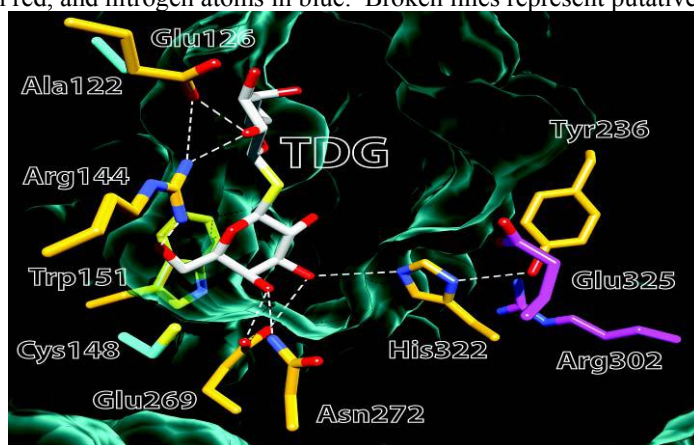


Figure 5. Cytoplasmic view of the active site in double-Trp LacY. TDG is shown as green sticks, and side chains forming H bonds with TDG are in yellow. Broken lines represent likely H bonds. Ala122 and Cys148, which are close to TDG but do not make direct contact, are shown in cyan. Glu325 and Arg302 are purple. The green, felt-like area represents the Van der Waals lining of the cavity. Note the narrow opening on the periplasmic side.

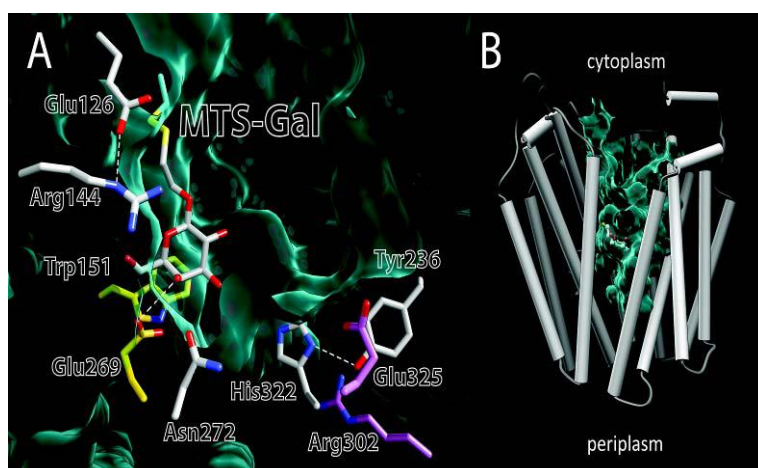


Figure 6: Crystal structure of single-Cys122 LacY with covalently bound MTS-Gal. (A) Side chains are shown as sticks; those in yellow (Glu269 and Trp151) make direct contact with the galactopyranosyl ring of MTS-Gal covalently bound to a Cys at position 122. Side chains in gray are not sufficiently close to make contact with the galactopyranosyl ring. Glu325 and Arg302 (in purple) are involved in H^+ transport. The green, felt-like area represents the Van der Waals lining of the cavity. Note that the periplasmic side is closed. (B) Structure of single-Cys122 LacY with covalently bound MTS-Gal viewed from the side. Helices are depicted as rods, and MTS-Gal is shown as spheres colored by atom type with carbon in green. The aqueous central cavity open to the cytoplasmic side is colored light green.

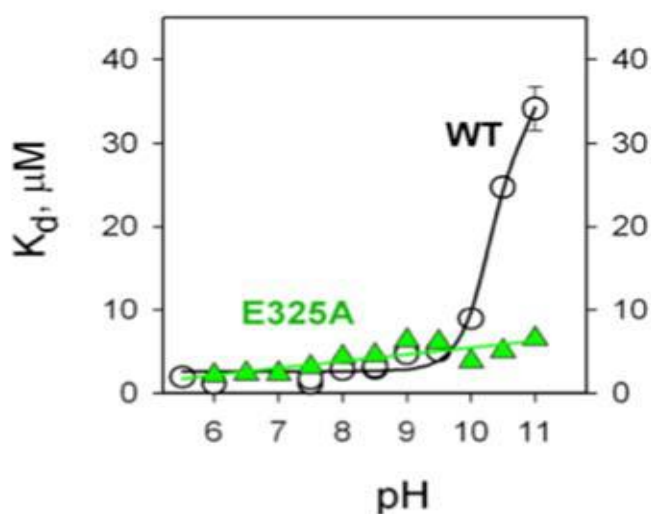


Figure 7: Effect of pH on the K_d^{app} for TDG binding to WT LacY (black) and the E325A mutant (green).

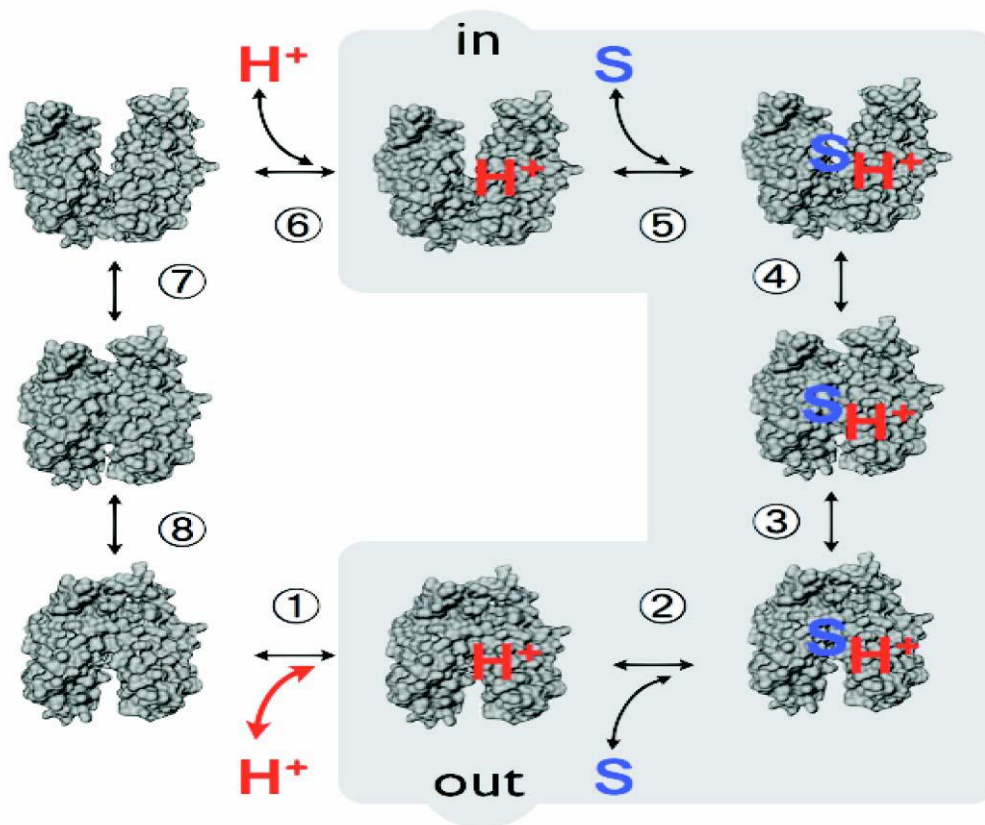


Figure 8: Kinetic scheme for galactoside/H⁺ symport, exchange and counterflow. Symport starts with protonation of LacY (step 1 or 6 for influx or efflux, respectively), which is required for high-affinity binding of lactose. Sugar binding to protonated LacY (steps 2 or 5) causes a conformational change to an occluded state (steps 3 or 4), which can relax to either side where sugar dissociates first (steps 2 or 5), followed by deprotonation (steps 1 or 6) and return of unloaded LacY via an apo occluded intermediate (steps 7 and 8). Exchange or counterflow involves only steps 2-5 (gray shaded area). Since LacY catalyzes symport in both directions, when symport is in the influx direction--step 1, protonation--the pK is very alkaline (~10.5), and step 6--deprotonation--must have a much lower pK for deprotonation to occur (i.e., Arg302 approximates protonated Glu325). However, in the efflux direction, the pKs of these steps are reversed.

Recent Trends in High Strength Steel Fibre Reinforced Concrete

by Yuri Ribakov, Member EUAS

Short Biography

Full Professor, Department of Civil Engineering, Faculty of Engineering, Ariel University, Ariel, Israel

Ph.D. 1998 – 2001 Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.

*M.Sc. 1995-1998** Department of Civil Engineering, Technion - Israel Institute of Technology, Haifa, Israel.*

B.Sc. 1984-1991 Faculty of Civil Engineering, Ukrainian Institute of Water Management Engineering, Rivne, Ukraine (with first class honors).

2014, 2010, 2009, 2003, 2002 Humboldt Research Fellow, Germany

2008 Visiting researcher, Faculty of Built Environment & Engineering, School of Urban Development, Queensland University of Technology, Brisbane, Australia.

2001 Visiting Researcher, Department of Civil, Structural and Environmental Engineering, State University of New York at Buffalo, Buffalo, NY, U.S.A.

Honors & Awards: 1999 Tuvia Netzer award – given for the research entitled “Influence of dampers on response of tall buildings to earthquakes”.

2000 Abraham and Miriam Gutwirth Research Award.

2013 Reviewing Excellence Award, Engineering Structures, Elsevier.

2014 Outstanding Reviewer Award, Engineering Structures, Elsevier.

Since 2017 – Active Member, EU Academy of Sciences (EUAS).

Since 2016 – Board of Directors, International Engineering and Technology Institute (IETI).

Since 2015 – Senior Member, International Engineering and Technology Institute (IETI).

Since 2010 – Member of the International Physics and Control Society (IPACS).

5 monographs, 13 chapters in edited books, about 90 papers in professional journals, more than 80 papers in proceedings of international conferences.

Effect of steel fibers on mechanical properties of high strength concrete

Steel fibre reinforced concrete (SFRC) became in the recent decades a very popular and attractive material in structural engineering because of its good mechanical performance. The most important advantages are hindrance of macrocracks' development, delay in microcracks' propagation to macroscopic level and the improved ductility after microcracks' formation. SFRC is also tough and demonstrates high residual strengths after appearing of the first crack. This paper deals with a role of steel fibres having different configuration in combination with steel bar reinforcement. It reports on results of an experimental research program that was focused on the influence of steel fibre types and amounts on flexural tensile strength, fracture behaviour and workability of steel bar reinforced high-strength concrete beams. In the frame of the research different bar reinforcements (2Ø6 mm and 2Ø12 mm) and three types of fibres' configurations (two straight with end hooks with different ultimate tensile strength and one corrugated) were used.

Three different fibre contents were applied. Experiments show that for all selected fibre contents a more ductile behaviour and higher load levels in the post cracking range were obtained. The study forms a basis for selection of suitable fibre types and contents for their most efficient combination with regular steel bar reinforcement.

Recent trends in high strength steel fibre reinforced concrete

High strength steel fibre reinforced concrete (HSSFRC) became in the recent decades a very popular material in structural engineering. High strength attracts designers and architects as it allows improving the durability as well as the aesthetics of a construction. As a result of increased application of HSSFRC, many experimental studies are conducted to investigate its properties and to develop new rules for proper design. One of the trends in HSSFRC structures is to provide their ductile behavior that is desired for proper structural response to dynamic loadings. An additional goal is to limit development and propagation of macro-cracks in the body of HSSFRC elements. HSSFRC is tough and demonstrates high residual strengths after appearance of the first crack. Experimental studies were carried out to select effective fibre contents as well as suitable fibre types, to study most efficient combination of fibre and regular steel bar reinforcement. Proper selection of other materials like silica fume, fly ash and super plasticizer has also high importance because of the influence on the fresh and hardened concrete properties. Using modern nondestructive testing techniques like acoustic emission and nonlinear ultrasound allows verification of most design parameters and control of HSSFRC properties during casting and after hardening. This paper presents a review of recent experimental results, obtained in the field HSSFRC and non-destructive testing. It compares the experimental data with provisions of existing codes and standards. Following this discussion and analysis, possible ways for developing modern design techniques for HSSFRC structures are emphasised.

Experimental Investigation of Full Scale Two-Layer Reinforced Concrete Beams

Two-layer beams (TLB), consisting of steel fibered high strength concrete (SFHSC) in the compression zone and normal strength concrete (NSC) in the tensile one, are studied experimentally. The current study is based on results of previous theoretical investigations and tests that showed high efficiency of such beams, carrying rather big bending moments. According to the previously developed concept, the fiber content for TLB should be calculated, corresponding to the required ductility level of an RC element. Following the results of a previous experimental study that were carried out to select the optimal fiber ratio, the current research is focused on testing full scale TLB. The study is aimed at experimental verification of the data related to interaction of concrete layers in TLB and proving the efficiency of two-layer bending element from beginning of loading and up to the

ultimate load stages, including collapse. Development of Poisson deformations was studied to compare them with those obtained in the previous study for cylindrical specimens. The SFHSC layer was cast after the NSC hardening to study the influence of separate casting technology that is more convenient for TLB production in real construction. Three identical specimens with constant fiber content, corresponding to the proper ductility level, were prepared and tested by four-point loading. The results demonstrate the role of fibers in a high strength concrete layer and form a basis for development of TLB design provisions.

Experimental Investigation of Continuous Two-Layer Reinforced Concrete Beam

Models and full scale statically determined two-layer beams (TLB), made of steel fibered high strength concrete (SFHSC) in the compression zone and normal strength concrete (NSC) in the tensile one, were previously tested by the authors. The present study is a further stage of these investigations that is focused on testing a continuous two span TLB with optimal steel fiber ratio like at the previous stages. This is the first experimental investigation of continuous TLB (CTLB). The study is aimed at testing the CTLB behavior under positive and negative bending moments in the span and above the middle support, respectively. An additional issue that is studied in the frame of this work is the influence of the bending moments' redistribution on the behavior of a CTLB. Like in the previous research stages, the interaction of concrete layers in a CTLB was studied to prove the efficiency of such beams for real structures. No cracks between the SFHSC and NSC layers were observed up to the ultimate limit state of the tested beam that demonstrates proper interaction between the layers. Results that are obtained in the present study enable to recommend CTLB for practical application as effective and economical continuous bending elements.

Recent 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 485 journal articles, 113 peer-reviewed conference papers, and 12 book chapters. Based on the Web of Science, his publications have over 13,750 citations, with an h-index of 57; based on Google Scholar, his publications have been cited over 17,900 times, with an h-index of 67.

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.

Experimental methods and large-scale atomistic simulations have been used to study the separate and coupled effects of energy loss to electrons and atomic nuclei on ion beam modification and radiation effects in materials. While grain growth in nanocrystalline materials is generally thermally activated, the growth can be driven by ion irradiation at much lower temperatures. Because of the temporal and spatial coupling of energy dissipation processes on the electronic and atomic structures, we have demonstrated that grain growth in nanocrystalline ceria and zirconia is dependent on the combined total energy loss to electrons and atomic nuclei. In the case of zirconia, this additive effect on grain growth is more efficient at 160 K than at room temperature. This work leads to new possibilities to control grain sizes and improve functionality of nanocrystalline oxides. We have similarly demonstrated that the temporal and spatial coupling of energy dissipation processes can lead to faster amorphization of zircon due to the additive effect of energy loss to electrons and atomic nuclei. These results have important implication for age-dating of natural zircon minerals and for the use of zircon as a waste form for the immobilization and disposal of plutonium in a geologic repository.

Silicon carbide (SiC) is an important wide-band gap semiconductor for high-temperature, high-power, and high-frequency applications. Moreover, its high corrosion, oxidation and radiation resistance make it a critical material with great potential for extremely harsh radiation environments. Using both experimental methods and large-scale atomistic simulations to study the effects of electronic energy loss, we have demonstrated that the energy transferred to the electrons of SiC from energetic ions via inelastic ionization can effectively heal pre-existing defects and restore the structural order. The threshold determined for this healing process reveals that it is activated at a relatively low electronic energy loss of 1.4 keV/nm, which is equivalent to the electronic energy loss for carbon ions at 850 keV. We have further shown that, when the energy loss to electrons and atomic nuclei are of comparable magnitude, the competitive effect between healing processes and defect production, due to electronic energy loss and elastic collisions between atomic nuclei, respectively, leads to a decrease in damage production that

is proportional to the ratio of the energy loss to electrons over the energy loss to atomic nuclei. These results provide a non-thermal approach to repair defects created by ion-implantation of SiC devices and will lead to improved control and performance predictions for SiC as either a functional material for device applications or a structural material for high-radiation environments. We have identified similar competitive effects between energy loss to electrons and atomic nuclei in several oxides under consideration for the immobilization of nuclear waste, and our results have critical implications for development of nuclear waste forms and for predicting the long-term performance of nuclear waste forms in a geologic repository.

Perovskite structured oxides, such as strontium titanate (SrTiO_3), are considered critical materials in the area of functional oxide electronics, with unexpected and emergent functionalities related to interfacial structures. Our integrated experimental and computational research has demonstrated that a colossal synergy occurs between inelastic energy loss by ions to electrons and pre-existing atomic defects created by elastic energy loss from low-energy ions in both single crystal SrTiO_3 and potassium tantalate (KTaO_3), resulting in the formation of nanometer-sized amorphous tracks, but only in the region with pre-existing defects. These pre-existing defects locally decrease the electronic and lattice thermal conductivities and increase the electron-phonon coupling, which locally increase the intensity of the thermal spike for each ion. This work identifies a major gap in understanding on the role of defects in electronic energy dissipation and electron-phonon coupling; it also provides insights for creating novel cylindrical interfaces and nanostructures to functionalize thin film structures, including tunable electronic, ionic, magnetic and optical properties.

Above a critical threshold in electronic energy loss, energetic heavy ions can create cylindrical ion tracks with concentric shell structures in many oxide ceramics. We have demonstrated that some of these concentric structures are metastable phases stabilized by local strain. Using advanced scanning transmission electron microscopy, coupled with density functional theory and atomistic simulations, our work has provided insights at sub-angstrom scale on the disordering induced variations in the local atomic environment and their effects on the electronic structure in these nanochannels. This research has revealed a remarkable enhancement in oxygen diffusivity in these cylindrical nanochannels that may be suitable for devices employing fast oxygen ion conductivity.

Theoretical Physics: New Contributions

by Dick Bedeaux, Member EUAS



Short Biography

Education and degrees

Master degree in Theoretical Physics, Utrecht University,
The Netherlands, November 1964.

PhD degree for a thesis on "The relation between the virial coefficients
and the scattering operator." Advisor Prof. Dr. N.G. van Kampen, Institute
for Theoretical Physics, Utrecht University, The Netherlands, May 1969

Positions

Research associate, Instituut Lorentz, University of Leiden, The Netherlands, 1972-1981.
Professor of Theoretical Physics, Norges Tekniske Hogskole, Trondheim, Norway, 1981-1983.
Professor of Physical Chemistry, University of Leiden, The Netherlands, 1984-2006, emeritus from
2006.

Professor II of Physical Chemistry, Norwegian University of Science and Technology, Trondheim,
Norway, 2003-2011, emeritus from 2011.

Publications and citation statistics, Aug. 2015

Google Scholar: Hirsch factor 47 (Citations since start: 7297 since 2010: 2498)

ISI Web of science: (without books): Hirsch factor 38 (Citations 5114)

Erdős number: 3

Total Publications: 285

Granted patent

S. Kjelstrup, T.V. Island, E. Saunar, and D. Bedeaux, Fremgangsmåte for optimalisering av
entropiproduksjon i en eller flere kjemiske reaktorer, Norsk patent nr. 311286, filed June 17 1998,
Accepted Nov.12, 2001

Prizes/Awards/Academy memberships

1996-: Foreign member of the Norwegian Academy of Technology

1997: Onsager medal

1997-: Fellow of the American Physical Society

1997-1998: Onsager professor, NTNU, Trondheim, Norway

1997-2005: Guest professor, University of Strathclyde, Glasgow, UK.

2007-2008: Extraordinary sabbatical at Centre of Advanced Studies, Oslo.

2011-: Member of the Royal Norwegian Society of Science and Letters

2015-: Member of the EU Academy of Sciences

Research Grants

- Co-recipient, with J.V. Sengers, US, and P. Mazur, NL, of a NATO travel grant, 1976-1979

- Co-recipient, with R. Greef, UK, and J. Vlieger, NL, of a NATO travel grant, 1983-1985

- Co-recipient, with J.M. Rubi, Spain, of a EC contract for Guest Scientists, 1985-1990

- Co-recipient, with T. Ytrehus, Norway, of a NATO travel grant, 1989-1992

- Co-recipient, with P. Schaaf, France, and J.M. Rubi, Spain, of an EU Laboratory Twinning Contract, 1991-1994
- Participant in the EU Network on Thermodynamics of Complex Systems,
- Coordinator B. Lavenda, University of Camerino, Italy, 1993-1998
- Co-recipient, with A.I. Murdoch, Glasgow, UK, of a SERC research grant, 1994-1995
- Co-recipient, with K. Kitahara, of a research grant from the Japanese government, 1998 -2002
- Recipient of a research grant from the Research Council of Norway, 2003-2005
- Participant in a Storfork grant to Signe Kjelstrup, Research Council of Norway, 2005-2010

Management experience

- Chairman of the Department of Physical and Macromolecular Chemistry, University of Leiden, The Netherlands, 1986-2002
- Member, secretary and chairman of the Working Group on "Liquids and Interfaces" of the Dutch Research Organization S.O.N. in Chemistry, 1990-1997
- Chairman of the Department of Chemistry, University of Leiden, The Netherlands, 1993-1995
- Member of the Board of the Leiden Institute of Chemistry, University of Leiden, The Netherlands, 1995 -1998

Publications and abstracts of Dick Bedeaux in 2016

E. Kustova, M. Nabokova, S. Kjelstrup and D. Bedeaux,

Heat and mass transfer in reacting mixtures: Molecular dynamics and kinetic theory approaches,

AIP Conference Proceedings 1786 (2016) 070007; doi: 10.1063/1.4967583

Abstract.

Transport properties of a binary H₂-H mixture with strongly-non-equilibrium dissociation reaction are studied on the basis of two approaches: kinetic theory and molecular dynamics. The gas in the thermostat under the action of temperature gradient is considered. Mass diffusive and measurable heat flux are obtained in the non-equilibrium molecular dynamics simulations; the transport coefficients are extracted from the fluxes using the constitutive equations given by irreversible thermodynamics. For the same conditions, the transport coefficients and the corresponding fluxes are calculated using the modified Chapman–Enskog method for the rarefied flows with non-equilibrium chemical reactions. While the qualitative agreement between the results obtained using the two approaches is found, quantitative differences are however noticeable. The discrepancy in the heat conductivity coefficient is not large but is significant for diffusion coefficients. Possible sources of discrepancies are discussed.

S Kjelstrup, R Skorpa, SK Schnell, D Bedeaux

Computing properties of the hydrogen dissociation reaction in and away from equilibrium,

Molecular Simulations 42 (2016) 1343-1355.

Abstract

We study the dissociation of hydrogen from molecule to atoms and show how we can compute thermodynamic and transport properties of both species in a mixture under non-ideal conditions. The small system method can be used to sample fluctuations of a few atoms or molecules in a small volume element, and gives fast access to accurate thermodynamic data of mixtures that are non-ideal. From the

results of equilibrium and non-equilibrium molecular dynamics simulations of the dissociation of hydrogen in a thermal field, we compute coefficients for transport of heat and mass for the gas mixture (0.0052 g cm^{-3}) at average temperature 10400 K. We show that the interdiffusion coefficient, the thermal conductivity and the Dufour effect are significantly affected by the presence of the reaction.

CD Daub, J Tafford, S Kjelstrup, D Bedeaux and F Bresme,

Molecular alignment in molecular fluids induced Q1 Q2 by coupling between density and thermal gradients,

Phys. Chem. Chem. Phys., 18 (2016) 12213-12220, DOI: 10.1039/C6CP01231K

Abstract

We investigate, using non-equilibrium molecular dynamics simulations and theory, the response of molecular fluids confined in slit pores under the influence of a thermal gradient and/or an applied force. The applied force which has the same functional form as a gravitational force induces an inhomogeneous density in the confined fluid, which results in a net orientation of the molecules with respect to the direction of the force. The orientation is qualitatively similar to that induced by a thermal gradient. We find that the average degree of orientation is proportional to the density gradient of the fluid in the confined region and that the orientation increases with the magnitude of the force. The concurrent application of the external force and the thermal gradient allows us to disentangle the different mechanisms leading to the thermal orientation of molecular fluids. One mechanism is connected to the density variation of the fluid, while the second mechanism can be readily observed in molecular fluids consisting of molecules with mass or size asymmetry, even in the absence of a density gradient, hence it is connected to the application of the thermal gradient only.

R Rurali, L Colombo, X Cartoixa, Ø Wilhelmsen, TT Trinh, D Bedeaux and S Kjelstrup,

Heat transport through a solid–solid junction: the interface as an autonomous thermodynamic system,

Communication: Phys. Chem. Chem. Phys. 18 (2016) 13741, DOI: 10.1039/c6cp01872f

Abstract

We perform computational experiments using nonequilibrium molecular dynamics simulations, showing that the interface between two solid materials can be described as an autonomous thermodynamic system. We verify the local equilibrium and give support to the Gibbs description of the interface also away from the global equilibrium. In doing so, we reconcile the common formulation of the thermal boundary resistance as the ratio between the temperature discontinuity at the interface and the heat flux with a more rigorous derivation from nonequilibrium thermodynamics. We also show that thermal boundary resistance of a junction between two pure solid materials can be regarded as an interface property, depending solely on the interface temperature, as implicitly assumed in some widely used continuum models, such as the acoustic mismatch model.

Thermal rectification can be understood on the basis of different interface temperatures for the two flow directions.

H Qian, S Kjelstrup, AB Kolomeisky and D Bedeaux,

Entropy production in mesoscopic stochastic thermodynamics: nonequilibrium kinetic cycles driven by chemical potentials, temperatures, and mechanical forces,

J. Phys.: Condens. Matter 28 (2016) 153004 (13)

Abstract

Nonequilibrium thermodynamics (NET) investigates processes in systems out of global equilibrium. On a mesoscopic level, it provides a statistical dynamic description of various complex phenomena such as chemical reactions, ion transport, diffusion, thermochemical, thermomechanical and mechanochemical fluxes. In the present review, we introduce a mesoscopic stochastic formulation of NET by analyzing entropy production in several simple examples. The fundamental role of nonequilibrium steady-state cycle kinetics is emphasized. The statistical mechanics of Onsager's reciprocal relations in this context is elucidated. Chemomechanical, thermomechanical, and enzyme-catalyzed thermochemical energy transduction processes are discussed. It is argued that mesoscopic stochastic NET in phase space provides a rigorous mathematical basis of fundamental concepts needed for understanding complex processes in chemistry, physics and biology. This theory is also relevant for nanoscale technological advances.

Ø Wilhelmsen, T T Trinh, A Lervik, VK Badam, S Kjelstrup and D Bedeaux,

A Coherent Description of Transport across the Water Interface: from Nanodroplets to Climate Models,

Phys.Rev. Phys. Rev. E 93 (2016) 032801

Abstract

Transport of mass and energy across the vapor-liquid interface of water is of central importance in a variety of contexts such as in climate models, weather forecasts and power plants. We provide a complete description of the transport properties of the vapor-liquid interface of water with the framework of nonequilibrium thermodynamics. Transport across the planar interface is then described by 3 interface transfer coefficients where 9 more coefficients extend the description to curved interfaces. We obtain all coefficients in the range 260-560 K by taking advantage of water evaporation experiments at low temperatures, nonequilibrium molecular dynamics with the TIP4P/2005-model at high temperatures, and square gradient theory to represent the whole range. Square gradient theory is used to link the region where experiments are possible (low vapor pressures) to the region where nonequilibrium molecular dynamics can be done (high vapor pressures). This enables a description of transport across the planar water interface, interfaces of bubbles, droplets, as well as interfaces of water-structures with complex geometries. The results are likely to improve the description of evaporation and condensation of water at widely different scales; they open a route to improve the understanding of nanodroplets on a small scale and the precision of climate models on a large scale.

Performance of Novel Nanocomposites for Optoelectronic and Biomedical Applications

by S. C. Tjong

Short Biography

Professor, Department of Physics and Materials Science

City University of Hong Kong

Prof. S C. Tjong graduated B.Sc. in Physics from National Taiwan University in 1973, followed by postgraduate studies in materials science at The University of Manchester (United Kingdom). He received M.Sc. and Ph. D. degrees in 1974 and 1976, respectively. After graduating from the University of Manchester, he worked as a materials engineer in China Steel Corporation (Taiwan) for nearly two years. He then went to the U.S.A as a Visiting Scientist at the Materials Science and Engineering Program, University of Texas at Austin, and Case Center for Electrochemical Sciences, Case Western Reserve University with famous electrochemist Professor E. B. Yeager. The research topics were related to the corrosion behavior of stainless steels welded by homopolar techniques (at Texas), and the fundamental mechanisms responsible for the passivation of Fe-based alloys using electrochemical, Raman and surface analytical techniques (at Case Western). Thereafter, he joined National Su Yat-Sen University (Taiwan) as an Associate professor and professor in materials engineering.

He supervised research students on the development of Fe-Mn-Al alloys for substituting chromium-based stainless steels. This was due to chromium element being considered as a strategic and scarce material at that period. He made contribution to the understanding of the structure, monotonic and cyclic (fatigue) mechanical properties as well as the corrosion properties of such alloys. He also conducted several consultancy projects with governmental agencies and the industrial sectors. Prior to joining the Department of Physics and Materials Science, City University of Hong Kong in 1990, he was employed as a Principal Scientist, Council for Mineral Technology, South Africa. The area of research was focused on the use of platinum group metals (Pt, Pd and Ru) for enhancing corrosion resistance of the Fe-Cr alloys. Currently, he is a professor at the City University of Hong Kong. Prof. Tjong has published over 370 SCI papers with 10,093 citations and an h-index of 52 (SCI), and 14,044 citations in Goggle with an h-index of 61, as well as six books. These books are:

(1) S. C. Tjong, "Nanocrystalline Materials: Their Synthesis-Structure-Property Relationships and Applications", Elsevier, 2006, ISBN 0-080-44697-3.

(2) S. C. Tjong, "Carbon Nanotube Reinforced Composites: Metal and Ceramic Matrices", Wiley VCH, 2009, ISBN 978-3-527-40892-4.

(3) S. C. Tjong, "Advances in Biomedical Science and Engineering", Bentham, 2009, ISBN978-1-60805-040-6.

(4) S. C. Tjong, Y.W. Mai, "Physical Properties and Applications of Polymer Nanocomposites", Woodhead Publishing (Elsevier), 2010, ISBN 978-1-84569-672-6.

(5) S. C. Tjong, "Polymer Composites with Carbonaceous Nanofillers: Properties and Applications", Wiley-VCH, 2012, ISBN 978-3-527-41080-4.

(6) S. C. Tjong, "Nanocrystalline Materials", 2nd Ed., Elsevier, 2014, ISBN 9780-1240-77966.

1. L. X. He and S. C. Tjong, Nanostructured transparent conductive films: Fabrication, characterization and applications, *Materials Science and Engineering R-Reports*, Vol. 109, pp. 1-101, 2016.

The need of ultimately thin, mechanically very strong and flexible transparent conductive electrodes for the indium tin oxide (ITO) replacement is growing as new technologies and devices such as touch screens, flexible displays, solar cells and OLEDs emerge rapidly in recent years. This requires the development and use of advanced functional materials having low-cost and environmental friendly processing techniques. Graphene, single-walled carbon nanotubes (SWNTs) and metallic nanowires (NWs) with unique properties have been explored as the alternatives for replacing brittle and expensive ITO. In particular, there is great interest in mass production of high quality and large-area graphene films for transparent conducting film (TCF) applications. The chemical vapor deposition (CVD) process is favored for the synthesis of large-area, high-quality graphene because of its compatibility with thin film processing facilities. CVD-grown graphene film on metal substrate generally exhibits polycrystalline domains having a high density of grain boundaries. After deposition, metal substrate should be removed, and graphene is transferred onto an insulating substrate for practical applications. Transfer processes introduce unavoidable surface impurities, cracks and excessive wrinkles in graphene. The presence of impurities, grain boundaries, structural defects and wrinkles can have an adverse effect on its optoelectronic performance. The complicated transferring process increases the production cost of graphene.

Liquid phase exfoliated-graphene synthesis is relatively simple for dispersing and exfoliating graphite flakes under sonication in water or organic solvents in the presence or absence of surfactants. However, most solvents are toxic, and graphene yield of this technique is relatively low. Furthermore, surfactants are difficult to remove from graphene, and the use of sonication, especially for long periods, can reduce the size of the resultant graphene sheets. Although chemical oxidation of graphite flakes in strong oxidizers can produce graphene oxide (GO) in large quantities. Additional chemical reduction or thermal annealing is needed to convert GO into conductive reduced graphene oxide (RGO) having a defective structure. Thus RGO is used in less demand applications such as defrosting heaters and supercapacitors. The electrical conductivity of RGO can be markedly improved by hybridizing with metallic nanowires to form nanocomposites.

As synthesized SWNT thin films consist of about 1/3 metallic-tubes and 2/3 semiconducting-tubes. The overall properties are related to many parameters including average tube length, tube diameter, abundance of m-SWNTs, impurities, etc. The quality of SWNTs plays a critical role since the presence of impurities and a large number of nanotube junctions can have an adverse effect on their optoelectronic performance. SWNTs generally contain metallic catalyst particles, fullerene and other carbonaceous impurities. Metallic catalysts can lead to light absorption, reducing optical transparency of the TCFs greatly. The purification procedures for removing these impurities and subsequent material examination techniques are required for examining purified CNTs. These will increase the production cost of SWNT-based TCFs.

As recognized, a high performance electrode should maintain a low sheet resistance and a high optical transmittance, corresponding to a high value of figure of merit (FOM). Silver nanowire-(AgNW) based TCFs have shown promise in rivaling ITO in sheet resistance, optical transparency and FOM values. The low sheet resistance and high haze of AgNW networks are particularly suitable for making transparent electrodes of solar cells. Finally, transparent conducting electrodes based on metallic nanowires can be fabricated at much lower cost using

solution processing techniques. Metallic nanowires can be easily dispersed into inks for forming TCFs. The ink processing is compatible with current industrial solution-based processes, such as roll-to-roll and rod coating production.

2. L. X. He and **S. C. Tjong**, Aqueous graphene oxide-dispersed carbon nanotubes as inks for the scalable production of all-carbon transparent conductive films, Journal of Materials Chemistry C, Vol. 4, pp. 7043-7051, 2016.

We report the utilization of aqueous graphene oxide (GO)-dispersed multi-walled carbon nanotubes (MWNTs) as the inks for simple, fast, and industrially scalable fabrication of transparent conductive films (TCFs) on a large scale. The GO–MWNT inks were rod-coated on uniform thin films, which were then chemically reduced by hydroiodic acid (HI) into reduced graphene oxide (RGO)–MWNT TCFs. We show how to utilize GO to make uniform dispersions of MWNTs in water, and how to optimize the wetting and rheological properties of the dispersion for coating and drying without dewetting. Treatment with HI yielded films with good electro-optical performance. Evaluation of the figure of merit (FOM) indicates that the RGO–MWNT film is superior to RGO, MWNT and un-doped single-walled carbon nanotube (SWNT) films. The use of the RGO–MWNT composite film as a transparent heater for defrosters is then demonstrated. Further scientific studies will pave the way for the deployment of GO–MWNT inks for commercial applications.

3. K. W. Chan, C. Z. Liao, H. M. Wong, K. W. Yeung and **S. C. Tjong**, Preparation of polyetheretherketone composites with nanohydroxyapatite rods and carbon nanofibers having high strength, good biocompatibility and excellent thermal stability, RSC Advances, Vol. 6, pp. 19417–19429, 2016.

In recent years, research in the development of polymeric materials for orthopedic implants has become ever more important because the global demand of biocompatible implants has been steadily increasing. Bioinert polyetheretherketone (PEEK) is typically reinforced with bioactive hydroxyapatite microparticles. However, the tensile strength of conventional PEEK/hydroxyapatite microcomposites falls sharply with increasing filler loading. To address low strength and high filler loading issues, nanohydroxyapatite rods (nHA) and carbon nanofibers (CNF) were employed to reinforce PEEK. In this study, molded-grade PEEK pellets, nHA and CNF fillers were melt-mixed and injection molded to form PEEK/nHA and hybrid PEEK/nHA–CNF nanocomposites. Tensile test results showed that elastic modulus of PEEK/nHA nanocomposites increases with increasing nHA content. The PEEK/9.3 vol% nHA nanocomposite exhibited higher tensile strength than that of a conventional HAPEX microcomposite. Thermogravimetric measurements indicated that the nHA addition improves the thermal stability of PEEK. Thus, the PEEK/9.3 vol% nHA nanocomposite that had good mechanical, thermal and biological performances was an attractive biomaterial for use in maxillofacial surgery. Furthermore, the tensile property of the PEEK/15vol% nHA–1.9vol% CNF nanocomposite compared favorably with that of human cortical bones. The results of biomineralization, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT), 2-(4-iodophenyl)-3-(4-nitrophenyl)-5-(2,4-disulfophenyl)-2H-tetrazolium (WST-1) assays and alkaline phosphatase (ALP) also showed that the PEEK/15vol% nHA and PEEK/15vol% nHA–1.9 vol% CNF nanocomposites exhibited excellent bioactivity and biocompatibility. The ALP assay showed good activity of osteoblast cells on the composite specimens with high nHA content. Moreover, CNF addition further increased the ALP activity of PEEK/15 vol% nHA nanocomposites.

4. C. Liu, H. M. Wong, K. W. Yeung and **S. C. Tjong**, Novel electrospun polylactic acid

nanocomposite fiber mats with hybrid graphene oxide and nanohydroxyapatite reinforcements having enhanced biocompatibility, *Polymers*, Vol. 8. pp. 287 (1) -287 (19), 2016.

Graphene oxide (GO) and nanohydroxyapatite rod (nHA) of good biocompatibility were incorporated into polylactic acid (PLA) through electrospinning to form nanocomposite fiber scaffolds for bone tissue engineering applications. The preparation, morphological, mechanical and thermal properties, as well as biocompatibility of electrospun PLA scaffolds reinforced with GO and/or nHA were investigated. Electron microscopic examination and image analysis showed that GO and nHA nanofillers refine the diameter of electrospun PLA fibers. Differential scanning calorimetric tests showed that nHA facilitates the crystallization process of PLA, thereby acting as a nucleating site for the PLA molecules. Tensile test results indicated that the tensile strength and elastic modulus of the electrospun PLA mat can be increased by adding 15wt% nHA. The hybrid nanocomposite scaffold with 15wt% nHA and 1wt% GO fillers exhibited higher tensile strength amongst the specimens investigated. Furthermore, nHA and GO nanofillers enhanced the water uptake of PLA. Cell cultivation, MTT and alkaline phosphatase tests demonstrated that all of the nanocomposite scaffolds exhibit higher biocompatibility than the pure PLA mat, particularly for the scaffold with 15 wt % nHA and 1wt %GO. Therefore, novel electrospun PLA nanocomposite scaffold with 15 wt% nHA and 1wt% GO possessing a high tensile strength and modulus, as well as excellent cell proliferation is a potential biomaterial for bone tissue engineering applications.

5. C. Liu, J. Shen, K. W. K. Yeung and **S. C.Tjong**, Development and antibacterial performance of novel polylactic acid-graphene oxide-silver nanoparticle nanocomposite mats prepared by electrospinning, *ACS Biomaterials Science & Engineering*, DOI: 10.1021/acsbiomaterials.6b00766.

Antibacterial nanomaterials have attracted great interest in recent years, especially with an increase in antibiotic resistance of microbial organisms. We have developed novel PLA-based fibrous mats with GO-Ag hybrid nanofillers through electrospinning for minimizing bacterial attachment and growth for biomedical applications. Polylactic acid (PLA) exhibits low tensile strength as well as no bactericidal ability. To enhance its tensile and bactericidal performances, 1 wt% graphene oxide (GO), and 1–7 wt% silver nanoparticle (AgNP) are incorporated into the PLA matrix. For comparison, electrospun PLA-1wt% GO and PLA-AgNP nanocomposites have also been prepared. The morphological, mechanical and thermal properties as well as bactericidal activities of electrospun PLA-based nanocomposite fibrous mats have been investigated. Tensile tests show that the addition of 1 wt % GO or 1–7 wt % AgNPs to PLA leads to a drastic increase in its elastic modulus. Further enhancements in tensile modulus and strength of PLA can be obtained by adding GO-AgNP nanohybrids. Agar disk diffusion test results indicate that the PLA-1wt% GO nanocomposite has no inhibition zones against *E. coli* and *Staphylococcus aureus* (*S. aureus*). However, GO nanofillers with lateral width of micrometer range act as effective anchoring sites for AgNPs. Thus, PLA-1wt% GO-(1–7) wt% Ag hybrid fibrous mats exhibit excellent antibacterial effect against *E. coli*, while the PLA-1wt% GO-Ag mats with higher AgNP loadings show bacterial inhibition toward *S. aureus*. The bactericidal effects of PLA-1wt% GO-(1–7)%Ag hybrids are studied and analyzed using live/dead fluorescent imaging assay, quantitative antibacterial efficacy test, SEM examination, and residual oxygen species measurement. Our work highlights the development of electrospun nanocomposite mats as promising antibacterial materials for biomedical applications and systematically depicts the bactericidal mechanism of PLA-GO-Ag nanocomposites.

The Complexity of Theorem-Proving Procedures

by Stephen Cook, Member EUAS

Short Biography

University Professor Emeritus

Department of Computer Science- University of Toronto

B.S. (Math) University of Michigan, Ann Arbor, 1961

S.M. (Math) Harvard University, 1962

Ph.D.(Math) Harvard University, 1966

Some Awards and Honours

A.M. Turing Award (October 1982)

Fellow, Royal Soc. of Canada (Inducted May, 1984)

Member, National Academy of Sciences (United States) (Elected to membership April, 1985)

Member, American Academy of Arts and Sciences (Elected to membership May, 1986)

Plenary Speaker, International Congress of Mathematicians, 1990 1995, 1999 Fellow, Royal Soc. of London

(Elected May, 1998) CRM/Fields Institute Prize, 1999

Fellow of the Fields Institute, June, 2002.

2006 John L. Synge Award, Royal Society of Canada

2008 Bernard Bolzano Honorary Medal for Merit in the Mathematical Sciences, awarded by the Academy of Science of the Czech Republic.

2008 Fellow of the ACM

2013 Gerhard Herzberg Canada Gold Medal for Science and Engineering 2015 Officer of the Order of Canada

2016 BBVA Frontiers of Knowledge Award in Information and Computer Technologies

Member, EU Academy of Sciences 2016

a. Research Endeavours

My major research areas are computational complexity and proof complexity.

b. Research Awards (grants, contracts, fellowships) during past 5 years

NSERC Operating Grant, April 1, 2011 to March 31, 2018, \$96,000/year

Herzberg Gold Medal Award (NSERC) April 1, 2013 to March 31, 2018, \$104,000/year

Soundness and Completeness of an Axiom System for Program Verification

Stephen A, Cook

SIAM JOURNAL ON COMPUTING, Vol 7 No, 1 (Feb. 1978).

Abstract. A simple ALGOL-like language is defined which includes conditional, while, and procedure call statements as well as blocks. A formal interpretive semantics and a Hoare style axiom system are given for the language. The axiom system is proved to be sound, and in a certain sense complete, relative to the interpretive semantics. The main new results are the completeness theorem, and a careful treatment of the procedure call rules for procedures with global variables in their declarations.

The Relative Efficiency of Propositional Proof Systems

Stephen A Cook and Robert A Reckhow

The Journal of Symbolic Logic

Volume 44, Number 1, March 1979

Summary: We are interested in studying the length of the shortest proof of a propositional tautology in various proof systems as a function of the length of the tautology. The smallest upper bound known for this function is exponential, no matter what the proof system. A question we would like to answer (but have not been able to) is whether this function has a polynomial bound for some proof system. Our results here are relative results.

We indicate that all standard Hilbert type systems (or Frege systems as we call them) and natural deduction systems are equivalent, up to application of a polynomial, as far as minimum proof length goes. We introduce *extended Frege* systems, which allow introduction of abbreviations for formulas. The most difficult result is Theorem 4.5, which states that all extended Frege systems, regardless of which set of connectives they use, are about equivalent, as far as minimum proof length goes. Finally in Section 5 we discuss the substitution rule, and show that Frege systems with this rule can simulate extended Frege systems.

Pebbles and Branching Programs for Tree Evaluation

STEPHEN COOK, University of Toronto

PIERRE MCKENZIE, Université de Montréal

DUSTIN WEHR and MARK BRAVERMAN, University of Toronto

RAHUL SANTHANAM, University of Edinburgh

ACM Transactions on Computation Theory, Vol 3, No. 2, Article 4, Publication date January 2012.

We introduce the *tree evaluation problem*, show that it is in **LogDCFL** (and hence in **P**), and study its branching program complexity in the hope of eventually proving a superlogarithmic space lower bound. The input to the problem is a rooted, balanced d -ary tree of height h , whose internal nodes are labeled with d -ary functions on $[k] = \{1, \dots, k\}$, and whose leaves are labeled with elements of $[k]$. Each node obtains a value in $[k]$ equal to its d -ary function applied to the values of its d children. The output is the value of the root. We show that the standard black pebbling algorithm applied to the binary tree of height h yields a deterministic k -way branching program with O states solving this problem, and we prove that this upper bound is tight for $h = 2$ and $h = 3$. We introduce a simple semantic restriction called *thrifty* on k -way branching programs states solving the Boolean problem “determine whether the root has value 1”, and prove that this bound is tight for $h = 2, 3, 4$. We also prove that this same bound is tight for unrestricted nondeterministic k -way branching programs solving the Boolean problem for $h = 2, 3$.

The Complexity of Theorem-Proving Procedures

Stephen A. Cook Proc. Third Annual ACM Symposium on Theory of Computing (STOC 3), 1971

Summary

It is shown that any recognition problem solved by a polynomial time-bounded nondeterministic Turing machine can be “reduced” to the problem of determining whether a given propositional formula is a tautology. Here “reduced” means, roughly speaking, that the first problem can be solved deterministically in polynomial time provided an oracle is available for solving the second. From this notion of reducible, polynomial degrees of difficulty are defined, and it is shown that the problem of determining tautologyhood has the same polynomial degree as the problem of determining whether the first of two given graphs is isomorphic to a subgraph of the second. Other examples are discussed. A method of measuring the complexity of proof procedures for the predicate calculus is introduced and discussed.

Accurate Measurements of Sea-Surface Temperatures from Satellite Infrared Radiometers

by Peter Minnett, Member EUAS

Short Biography

*Professor of Ocean Sciences, Rosenstiel School of Marine and Atmospheric Science
University of Miami, Miami, Florida, USA*

Oxford University, UK, B.A. in Natural Science, 1973

Southampton University, UK, M.Sc. in Oceanography, 1975

Southampton University, UK, Ph.D. in Oceanography, 1978

Dr. Minnett is currently Professor of Ocean Sciences at the Rosenstiel School of Marine and Atmospheric Sciences of the University of Miami in the USA, where he also serves as Speaker of the School Council. He has also served as Chair of Meteorology and Physical Oceanography at the Rosenstiel School. His career includes posts at the Christian-Albrechts University, Kiel in Germany; the Rutherford Appleton Laboratory, UK; at the NATO Undersea Research Center in Italy, and Brookhaven National Laboratory in the USA. He has also been on the Adjunct Faculty at North Carolina State University and the State University of New York at Stony Brook. He has participated in over twenty research cruises, including ten on research-icebreakers in the Arctic Ocean. Dr. Minnett's current research interests include infrared remote sensing of the ocean from satellites, including atmospheric effects on the radiative transfer in the infrared and the derivation of accurate sea-surface temperatures. He has recently stepped down as Chair of the Science Team of the international Group for High Resolution Sea-Surface Temperature (www.ghrsst.org). He also chaired a study group of the International Space Science Institute (ISSI) located in Bern, Switzerland, on the topic of generating Climate Data Records of SST from satellite measurements. In addition to satellite-based data, Dr Minnett uses ship-based infrared interferometry to study the physics of the upper ocean, including the properties of the ocean skin layer and air-sea exchanges, and he currently serves on the Scientific Steering Committee of the Surface Ocean – Lower Atmosphere Study (<http://www.solas-int.org/>). He is a member of several satellite instrument science teams and Science Advisory Groups in Europe as well as the USA. Dr. Minnett has published about a hundred peer-reviewed journal articles and over twenty book chapters and encyclopedia entries.

Past and current editorial responsibilities:

*Section Editor for “Satellite Remote Sensing”, Encyclopedia of Ocean Sciences, 3rd Edition.
Elsevier.*

Editorial Board of Remote Sensing of Environment.

Editorial Board of Surveys in Geophysics.

Associate Editor of Remote Sensing of Environment. (2008 - 2015)

*Editor of sections for “Oceans” and “Cryosphere” in Encyclopedia of Remote Sensing Springer
Science+Business Media. (2007- 2013)*

Editor Journal of Atmospheric and Oceanic Technology (2004-2007)

Editorial Board of Remote Sensing of Environment. (1999 - 2008)

In the late 18th Century, one of the first nautical depictions of the Gulf Stream was produced by Benjamin Franklin and Timothy Folger. Published as part of their chart of North Atlantic currents, it included acknowledgement not just of surface flow but also of temperature gradients across the Gulf Stream. However, it is only in more recent

times that the significance for global climate of the poleward heat transported by the ocean and the atmosphere has been realized.

There are now a number of widely recognized Essential Climatic Variables, which can be broadly grouped into atmospheric, terrestrial and oceanic categories. One of the key oceanic variables is sea surface temperature (SST), which is nearly everywhere greater than the atmospheric temperature immediately above it and as such provides a heating effect on the atmosphere. Thus, SST has a great impact on global climate, driving heat and moisture fluxes that contribute to the climate. SST is variable in both time and space, and is determined by a range of factors including integrated heat fluxes, turbulent mixing and advection. Difficulty in understanding the behavior of SST arises not only from these variables, but also from the differences in SST measurements using different methods taken at different depths. In particular, the interaction at the boundary between sea and atmosphere creates a thermal 'skin layer' on the surface of the ocean. Historically, SST refers to the temperature just below the surface, as measured by an in situ thermometer. But, the infrared emission from the ocean to the atmosphere, and the absorption by the ocean of atmospheric emission, occurs in the electromagnetic skin layer which extends into the water by only a fraction of a millimeter. Of comparable thickness, a thermal skin layer also exists on the aqueous side of the interface; the thermal skin layer is a result of the heat transfer between the ocean and the atmosphere. As the heat flow over nearly the entire ocean surface is from the water to the air, the temperature within the thermal skin layer - as measured by infrared radiometers on ships, aircraft and satellites - is generally cooler than the water beneath. The accuracy goal of SST for use in climate research is $\pm 0.1\text{K}$, with a stability target of $\pm 0.04\text{K}$ per decade. These are very stringent requirements and difficult not only to achieve, but also to demonstrate whether they have been attained.

The only feasible way of measuring the global distribution of SST is to use accurate radiometers on earth observation satellites. A scanning imaging radiometer with a wide swath on a polar orbiting satellite can provide global cover each day, or over two days, and a constellation of such satellites can provide appropriate coverage. Imaging radiometers on geostationary satellites can provide more rapid sampling, but of a disk of the earth centered at the sub-satellite point. A major problem with infrared remote sensing is the fact that clouds and aerosols prevent the propagation of the surface emission to the satellite height, with the result that only about 12% of all measurements over the ocean can be used to derive SST. This is not to say the oceans are ~88% cloud covered, but that ~88% of all pixels contain emission from clouds to a sufficient degree to contaminate the SST retrieval to an unacceptable level.

It is feasible to build infrared radiometers that can meet, in principle, the accuracy targets for measurements, but these are measurements at orbital heights. The key to accurate retrievals of SST from on-orbit measurements lies in the identification of pixels contaminated by emission from clouds and aerosols, so they can be discarded; and then the effects of molecules in the intervening atmosphere have to be corrected. These tasks are achieved by using measurements at different wavelength intervals in the infrared, and in the visible part of the spectrum for cloud screening during the sunlit part of every orbit. Thus, the satellite radiometers have multiple channels. To derive

surface temperatures, the wavelength intervals of the infrared channels are positioned where the atmosphere is relatively transmissive so that the satellite measurements contain information from the surface, even though it is modified by its propagation through the atmosphere.

SSTs derived from satellite measurements form one of the longest duration time series from earth observation satellites. The time series of multi-channel infrared measurement goes back to the early 1980's and in the period since then many algorithms have been developed to identify clouds in the satellite measurements, and in correcting the effects of the clear-sky atmosphere. However, none is perfect and situations are found where their objects are not met. Modifying algorithms to handle anomalous situations while not compromising their performance in the majority of conditions is a continuing topic of research.

It is difficult to demonstrate convincingly whether the target accuracies for climate monitoring and research have been met, or not. Identifying conditions under which the accuracies are poorer, and understanding the physical causes, is an important step in improving algorithms and thereby improving the accuracies of satellite-derived SSTs.

Throughout most of the period of satellite-derived SSTs, comparisons have been made with in situ measurements of temperature to evaluate the accuracy of the satellite SSTs. A very valuable source of in situ temperatures is free-drifting surface buoys deployed in the oceans to provide surface temperature and pressure measurements for weather forecasting. Currently there are about 1500 such drifters reporting their measurements and positions, now determined by GPS, several times per day (see <http://www.aoml.noaa.gov/phod/dac/index.php>). By comparing these temperatures with those from satellites, we can derive estimates of the accuracies of the satellite retrievals. For many years, the presumed accuracy of the drifter temperatures, $\pm 0.1\text{K}$, was seen as being a small contribution to the statistics of the differences, and thus the differences were ascribed entirely to errors and uncertainties in the satellite data. However, in recent years it has become apparent that the accuracies of the drifter temperature measurements are about $\pm 0.25\text{K}$, and this can no longer be ignored in assessing the accuracies of the satellite SSTs; it renders impossible the task of demonstrating whether the accuracies needed for climate research have been achieved. Furthermore, since the buoys are disposable and very rarely recovered, assessment of the accuracies after deployment are very difficult. Steps are underway to improve the accuracy of the thermometers prior to deployment and to assess the calibration degradation with time. But, even a perfect sub-surface temperature taken from a drifting buoy, at a depth of $\sim 20\text{cm}$ depending on the sea-state, does not provide an ideal measurement for comparison with SSTs derived from satellites. Differences between sub-surface temperatures and the skin SSTs result not only from the variable thermal skin effect, but also from temperature gradients caused by the absorption of solar radiation, particularly at times of low wind. This temperature stratification is referred to as the diurnal thermocline.

An alternative approach to assess the accuracy of the satellite SSTs is to match them with near-surface radiometric measurements. Thus, a comparison "like-with-like" is

being made. Beginning in the mid 1990's, We began to deploy very-well calibrated infrared spectro-radiometers on ships. The instruments, developed at the Space Science and Engineering Center at the University of Wisconsin-Madison, are Fourier-Transform infrared interferometers. To ensure accurate radiometry, these instruments include two large blackbody cavities for real-time calibration. The cavities are maintained at different temperatures and their emission is measured before and after the measurements of the oceanic and atmospheric emission in a continuous measurement cycle. Measurements of the atmospheric emission are necessary to correct for the small reflected component of the spectra taken when the gold-plated scan mirror of the instrument is directed at the sea surface. The instruments, called Marine-Atmospheric Emitted Radiance Interferometer (M-AERI), are mounted forward on the ships so the sea surface emission comes from an area ahead of the bow wave. The majority of deployments of the M-AERIs were on research ships, and these continue to be an important source of measurements in many of the world's oceans. Another option is to mount the instruments on cruise ships as these provide the opportunity for long duration deployments, up to several years, and for repeated measurements along the same track around the seasons, thus allowing comparative sampling in different conditions. Thus far, three ships of Royal Caribbean Cruises Ltd. have been and are being equipped with M-AERIs. To provide information about the conditions in which the ship to satellite comparisons are being made, instruments to monitor the marine meteorology are also mounted with the M-AERI's, and on some deployments radiosondes are launched just before the satellite overpass to characterize the atmospheric state.

My group routinely deploys three M-AERIs, along with much simpler filter radiometers that are also used by other groups working in this field, to provide data to improve the algorithms applied to the satellite data, and so there has to be a mechanism to ensure the shipboard measurements from multiple sensors are equivalent. To achieve this, the effectiveness of the internal calibration procedure of shipboard radiometers are frequently assessed by measurements in the laboratory at the Rosenstiel School of the emission from a water-bath blackbody calibration target. The target is a thin-walled copper cone immersed in a water bath the temperature of which can be maintained at programmed set-points to about 1 mK accuracy and stability of periods of hours. The inside of the cone is coated with high emissivity black paint. The calibrations of the reference thermometers in the water-bath are periodically checked against SI-reference standards, and a series of workshops have been held where the equivalence of laboratory blackbody targets can be assessed. The first three of these workshops were held at the Rosenstiel School which involved the US National Institutes of Science and Technology who contributed their reference Transfer Radiometer (TXR). The fourth workshop was held at the UK National Physical Laboratory in the summer of 2016 and their reference radiometer and blackbody targets were used. Through these workshops and the attention to ensuring good calibration of the shipboard radiometers used to determine the accuracy of skin SSTs derived from multiple satellite radiometers, the basis of generating Climate Data Records of SST from satellite radiometers is established through unbroken calibration chains to SI temperature standards.

New Developments on Advanced Structural Materials

by Chain T. Liu, Member EUAS

Short Biography

Professor C.T. Liu is a member of National Academy of Engineering (NAE), USA, a foreign member of Chinese Academy of Engineering, and an academician of Academia Sinica Taiwan. He is currently a University Distinguished Professor of City University of Hong Kong. He served as a Professor and Distinguished Research Professor at University of Tennessee between 2005 and 2009; a Chair Professor under the World Class Scholar Program at Hong Kong Polytechnic University, and a Distinguished Professor at Auburn University, USA between 2005 and 2010. He is a world leader in the field of intermetallic and metallic materials. He has done pioneer work on mechanistically understanding the brittle fracture in intermetallic alloys and intergranular fracture in noble refractory alloys, correlation of atomic structures of bulk metallic glasses (BMGs) with their unique mechanical properties, and hardening of ferritic steels with various nanoparticles. His innovative research has led to the design of new structural materials with superior mechanical properties for engineering applications. He has published close to 500 journal papers and been granted 29 US patents. In 1995, ISI had identified him as one of top five highly-cited authors in the materials field. Professor Liu has received numerous honours and awards, including Acta Metallurgica Gold Medal Award, the E.O. Lawrence Award (a US President award) from USDOE, Brown Engineering Alumni Award from Brown University, the first Henry J. Albert Award from IPMI, Fellow Awards from five professional societies – Japan Institute of Metals, the World Technology Network, TMS, ASM, and IPMI, four I•R 100 Competition Awards from Industrial Magazine USA. He was an editor and the Chief Editor of the International Journal of Intermetallics for almost 20 years.

Prof. CT Liu is a member of National Academy of Engineering (NAE) USA, an academician of Academia Sinica Taiwan, and a foreign member of Chinese Academy of Engineering (CAE). He is currently a University Distinguished Professor at City University of Hong Kong, Kowloon, Hong Kong. He is well known internationally for his outstanding contributions to the design and development of advanced structural materials. He did pioneer work on mechanistically understanding the brittle fracture in intermetallic alloys and intergranular fracture in noble refractory alloys, deriving new criteria based on thermodynamics and first-principles calculations to predict glass forming ability in metallic glasses, and designing strong and ductile bulk metallic alloys. All his innovative research and development have led to the design of new structural materials with superior mechanical and metallurgical properties for engineering applications. He has published more than 500 technical papers in archival journals, handbooks, and encyclopedia chapters. His papers have been cited extremely high by the materials community. In 1995, the Institute of Scientific Information (ISI) identified him as one of top five authors in worldwide ranking of highly cited authors in the materials and engineering field. He has received numerous honors and recognitions from academia, industrial, professional societies and government agencies, including the Acta Metallurgica Gold Medal Award in 2001, the E. O. Lawrence Award (a US President award) from US Department of Energy in 1998,

Brown Engineering Alumni Award from Brown University in 1998, the first Henry J. Albert Award from the International Precious Metals Institute (IPMI) in 1980, Fellows Awards from five societies – Japan Institute of Metals, the World Technology Network, TMS, ASM, and IPMI, four **I•R 100** Competition Awards from Industrial Research/Development Magazine USA, and many other awards and citations from US Department of Energy (DOE), NASA, Chinese Government Agencies, and Brown University.

Prof. Liu has been recognized as a world authority in the field of ordered intermetallics. His pioneer work on the effect of alloy stoichiometry and micro-doping on the ductility improvement of Ni₃Al greatly stimulated the interest in the study of ordered intermetallic alloys in the early 1980s. In 1988, he first discovered that nickel and iron aluminides are intrinsically ductile at ambient temperatures and that their poor ductility is essentially caused by moisture-induced hydrogen embrittlement at ambient temperatures. His innovative research has provided a new direction to the design of ductile intermetallic alloys for industrial use. He won two prestigious **I•R 100** Industrial Competition Awards for his development of new nickel and iron aluminide alloys. His recent paper on “polysynthetic twinned TiAl single crystals for high-temperature applications” just published in *Nature Materials*, 15, 876, 2016, which stimulated a great interest in the development of titanium aluminide alloys for high temperature applications

Prof. Liu worked on refractory alloys, including noble refractory metals, during this early career. He received four U.S. patents for his development of new precious metal alloys. The thorium-doped Ir-0.3% W alloy developed by him has been used as the major cladding material for many US space powder systems during the past three decades. Because of his innovative work, he was honored with the first Henry J. Albert Award given by IPMI in 1980, as well as many DOE and NASA citations and recognition.

In recent years, Dr. Liu has devoted his major research effort on two advanced materials: (1) Metallic Glasses and Bulk Metallic Glasses, and (2) High Entropy Alloys (HEAs). Bulk metallic glasses (BMGs) with amorphous structures possess many unusual properties for structural and functional use. In order to understand the glass forming ability, he and his team had developed a new expression to predict the glass forming ability for various Metallic glasses and BMGs. This paper was identified as one of mostly cited recent papers by the Institute for Scientific Information (ISI). Also, their innovative work on the development of new Fe-based BMGs with superior glass forming ability has been selected as one of the Top Physics Stories by American Physics Society in 2005. Also, he and his coauthors have identified the heterogeneous features in structures which contain loosely-bonded regions dispersed in the tightly-bonded matrix in MGs. All the unusual mechanical properties such as slip bands and delay yielding can be well explained by this heterogeneous model. Recently, his work on atomic structures and global mechanical properties of BMGs has been published in high-profile

journals, such as Physical Review Letters and Nature Materials in 2010.

For the past six years or so, he has devoted his research effort on high entropy alloys (HEAs), whose novel design concept has effectively extended alloy compositions from a traditional alloy regime to the hyperspace with multiple principle alloying elements. Recently, his group has discovered that a high density of intermetallic nanoparticles is able to successfully engineer into many HEAs being benefited from the guidance of thermodynamic calculations, resulting in a tremendous increase of strength combining with unexpected ductility. Also, the microband-induced plasticity (MBIP) effect is introduced during deformation of HEAs, realizing an effective combination with precipitation hardening. Based on this integrated strengthening mechanism, long-standing problem of deformation instability in high-strength materials is greatly eliminated by providing an exceptional strain hardening capability. As a result, the newly developed HEAs exhibit a simultaneously enhanced ductility at ultra-high strength level, which successfully defeats the intractable conflict of strength-ductility in traditional materials. This surprising finding change the general concept of previous materials that relying almost entirely on twinning-induced plasticity. (TWIP) or transformation-induced plasticity (TRIP) effects for ductility improvement, providing a new strategy to achieve the combined increase of strength and ductility. These findings are expected to have significant implications for the basic deformation mechanism and future development of HEAs as well as other advanced structural materials, such as superalloys and advanced steels.

Prof. Liu has been granted a total of 29 patents for his innovative work on development of new advanced structural materials. Also, he has published more than 500 papers on advanced metallic materials in material and physical journals. He was a funder as well as the Chief Editor of the *International Journal of Intermetallics* for more than 20 years, and had served as an editor and associated editors of many material journals. For his active collaboration and cooperation with China, he received a 2006 National Friendship Award from the Office of Foreign Affairs, Chinese State Council, and a 2007 National Award for International Scientific and Technological Collaboration from the National Office of Science and Technology Awards in China.

Experimental Physics of Interfaces

by Hans-Jürgen Butt, Member EUAS



Short Biography

1986 Diploma in Physics from the University of Hamburg, Germany

1989 PhD in Biophysics with the thesis "Time-resolved measurement of proton translocation by Bacteriorhodopsin supervised by Ernst Bamberg, Max Planck Institute of Biophysics, Frankfurt, Germany

1989-1990 Postdoc, Group of Prof. Dr. P.K. Hansma, University of California, Santa Barbara: Atomic force microscopy

1990-1996 Group of Prof. Dr. E. Bamberg, Max Planck Institute of Biophysics, Frankfurt

1995 Habilitation in Biophysical Chemistry at the University Frankfurt on Atomic force microscopy of biological objects

1996-2000 Associate Professor of Physical Chemistry at the University Mainz, Germany

2000-2002 Full-Professor of Physical Chemistry at the University of Siegen

2002 Director at the Max Planck Institute for Polymer Research Mainz

Appointments

2004 Honorary Professor at the University Mainz

2007-2008 Member Fachkollegium German Research Society (DFG) for physical chemistry of molecules, liquids, interfaces, theoretical chemistry

2007-2011 Member steering committee graduate school of Excellence "Materials Science in Mainz"

2007-2014 Member steering committee center of Excellence "Smart Interfaces" in Darmstadt

2007-2011 Chair of the German Colloid Society

2008-2014 Spokesperson International Max Planck Research School for Polymer Materials

2009 Council member International Association of Colloid and Interface Scientists (IACIS)

2009 Honorary Professor at the Technical University Darmstadt

2010-2016 Treasurer of the European Colloid and Interface Society (ECIS)

2015 President-Elect International Association of Colloid and Interface Scientists (IACIS)

2016 Member Fachkollegium of the German Research Society (DFG) for Polymer Research

2016 Senior member of the Gutenberg Academy of the University of Mainz

Prizes and Honors

1996 Heisenberg fellowship

2008 Tewkesbury Lecture in Melbourne, Australia

2008 ICI distinguished Lecturer, University of Edmonton, Alberta, Canada

2011 Lectureship Award, Division of Colloid & Surface Chemistry, Chemical Society of Japan

2013 ERC Advanced grant: Superamphiphobic Surfaces for Chemical Processing

2017 Member of EU Academy of Sciences

Overview

We study the structure and dynamics of soft matter interfaces. The scientific aim is a simple, comprehensive quantitative description of phenomena. This description should be based on fundamental physical laws. Major research topics are: super liquid-repellency, dynamics of wetting, surface forces, crystallization in confined space, colloids and granular matter. The methods used include scanning probe techniques, confocal microscopy, fluorescence correlation spectroscopy, light and X-ray scattering. To expand the range of length and time scales accessible, new methods are continuously developed to access shorter time and smaller length scales. Our goal is to solve fundamental questions, with the perspective of future applications. “Understanding” not only implies quantitative prediction. Full understanding implies being able to make new materials and devices based on this understanding. For this reason the department also includes materials science and even a synthesis group (currently on photoresponsive materials), although its core is experimental physics.

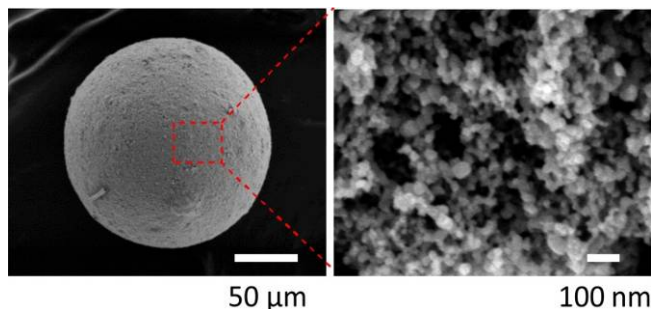
The goal of the department is also to produce creative, mature and independent scientists that conduct research in a highly interdisciplinary environment with cooperation partners worldwide. They are encouraged to use the knowhow and infrastructure at the Max Planck Institute and cooperate with other group leaders providing complementary expertise.

Super liquid repellency

Driven by the ERC advanced grant “Superamphiphobic surfaces for chemical processing” (started 2014) we study superliquid repellent surfaces. The general aim is control wetting by nanostructuring surfaces. Three examples illustrate the range of activities.

1. Using confocal microscopy we image water drops advancing on a superhydrophobic array of micropillars. In contrast to common belief, advancing and receding are fundamentally different processes. When advancing, the liquid surface gradually bends down until it touches the top face of the next micropillars. On the receding side, pinning to the top faces of the micropillars determines the apparent receding contact angle. Receding contact angle should be used for characterizing superliquid repellent surfaces rather than the advancing contact angle (Schellenberger et al., *Phys. Rev. Lett.* **2016**, *116*, 6101. Highlighted by *Nature Materials* **2016**, *15*, 376).
2. **Enhancing CO₂ capture using robust super amphiphobic membranes.** Gas membranes are used to exchange gas between the gaseous and the dissolved phase in a liquid. They are essential for many processes in chemical engineering. We aim to fabricate and test superamphiphobic gas membranes. The hope is that such membranes are more efficient than conventional gas membranes and that they reduce clogging and biofilm formation. As one important example we introduce superamphiphobic membranes for enhanced CO₂ absorption (Geyer et al., *Adv. Mater.* **2017**, *29*, 1603524.). The CO₂ capture rates of our membranes were enhanced by more than 20%.
3. **Particle factory: Fabrication of microparticles on superliquid repellent surfaces.** The almost contact-free interface between the liquid and a superamphiphobic surface may open up the opportunity for fabricating complex spherical particles (diameter 20-2000 μm). As a proof of principle we synthesized polymer microspheres without solvent and we produced TiO₂ supraparticles by evaporation of drops of dispersions (Wooh et al., *Adv. Mater.* **2015**, *27*, 7338) (Fig. 1).

Figure 1. Supraparticles consisting of a porous aggregate of TiO_2 nanoparticles prepared on a superoleophobic surface.



Dynamics of wetting

Although the wetting dynamics of pure, simple liquids is to some degree known, the wetting of more complex liquids such as solution, emulsions, dispersion, is far from being understood.

This is rather unfortunate because practically all liquids in our daily life or in industrial applications are complex. As a first step we study the dynamics of wetting of surfactant solutions. The dewetting behavior of surfactant solutions differs significantly from pure liquids due to the generation of Marangoni stresses near the three phase contact line (Henrich et al., *Soft Matter* **2016**, *12*, 7782). We have shown that surfactant solutions show a much stronger velocity dependence of the dynamic receding contact angle than comparable pure liquids. The process scales with the critical micelle concentration and is (to a first approximation) independent of the charge and molecular weight of the surfactant.

Surface forces

To measure surface forces at a pressure which exists in deep sea or during oil recovery, we designed an optical trapping setup. It allowed us to explore the interaction of a micrometer-sized glass bead and a solid glass wall up to 1 kbar. We are further interested in surface forces between very soft surfaces. Quantifying mechanical properties of soft or biological materials with Young's moduli below 100 kPa is difficult because in addition to adhesion and elasticity, surface stress plays a critical role. Until now, microscale contact of very soft materials has only been studied by static experiments with zero external loading. We combined colloidal probe atomic force microscopy and confocal microscopy to characterize the full force-indentation and force-contact geometry relationships during microindentation of soft silicone solids. We demonstrate that the widespread Johnson-Kendall-Roberts theory cannot predict the mechanical contact for such soft materials. With a simple analytical model, we illustrate that contributions of both solid surface stress and liquid surface tension need to be taken into account.

Atomic force microscopy of photovoltaic materials

Efficient charge extraction within solar cells depends on the optimization of the internal interfaces. In the case of perovskite solar cells, slow processes happening on timescales of seconds cause hysteresis in the current-voltage characteristics. We localized and investigated these slow processes with frequency modulation Kelvin probe force microscopy (FM-KPFM) on cross sections of planar methylammonium lead iodide perovskite solar cells. Upon illumination, space charge layers were forming at the interfaces to the methylammonium lead iodide layer within several seconds (Bergmann et al., *Nature Commun.* **2014**, *5*, 5001). To analyze the humidity sensitivity we performed in-situ scanning force microscope and in-situ X-ray diffraction measurements to track changes in the methylammonium lead iodide film morphology and crystal structure upon repeated exposure to a high relative humidity of 80%.

Fluorescence correlation spectroscopy in polymer and colloid science (K. Koynov)

Fluorescence correlation spectroscopy (FCS) is a sensitive and selective technique for

studying the mobility of fluorescent species, such as small molecules, macromolecules or nanoparticles, in various environments. It is based on monitoring fluctuations of the fluorescence intensity originating from species diffusing through a small illumination volume. The illumination volume is the “focus” of a confocal microscope. A correlation analysis of these fluctuations yields information on the diffusion coefficients of the species, their fluorescence brightness, concentration, etc. Commonly, these parameters are measured and used to assess the fluorescent species’ size, aggregation behavior, and interactions with other species. Alternatively, one can obtain information about the surrounding environment.

While initially developed as a tool in molecular and cell biology, during the last decade FCS has also become an established technique in polymer, colloid and interface science. In close cooperation with other groups from MPIP we are strongly contributing to this endeavor and apply FCS to address variety of research questions. Using FCS we analyze the polymers in dilute solutions, in porous media (Xie et al., *ACS Macro Lett.* **2016**, *5*, 190) or in the melt. We further try to understand how molecular traces or nanoparticles diffuse in inhomogeneous media.

Crystallization of soft matter in hard confinement

Understanding how, why and when polymers crystallize under confinement is a fundamental problem in polymer physics with important technological applications. Of central importance to this discussion is the origin of heterogeneous and homogeneous nucleation and their possible relation to the freezing of the local segmental dynamics at the liquid-to-glass temperature. Recent studies of polymer crystallization demonstrated that by confining polymers to small isolated volumes of anodic aluminum oxide (AAO) one can suppress heterogeneous nucleation in favor of homogeneous nucleation (Zardalidis et al., *Soft Matter* **2016**, *12*, 8124). This resulted to the first phase diagrams for confined semicrystalline polymers. We further explored the origin of “impurities” and of the polymer architecture.

Subsequently, these ideas were expanded to ice formation within the same AAO templates (Suzuki et al., *Nano Letters* **2015**, *15*, 1987). We found a transition from heterogeneous nucleation of hexagonal ice (I_h) to homogeneous nucleation of predominantly cubic ice (I_c) with decreasing pore diameter. These results lead to a phase diagram of water under confinement. It contains a (stable) predominant I_c form, a form known to exist only in the upper atmosphere.

Photoresponsive polymers

The development of polymers with switchable glass transition temperatures (T_g) can address scientific challenges, including the healing of cracks in high- T_g polymers and the processing of hard polymers at room temperature without using plasticizing solvents. Recently, we found that light can switch T_g of azobenzene-containing polymers (azopolymers) and induce reversible solid-to-liquid transitions of the polymers (Zhou et al., *Nature Chemistry* **2017**, *9*, 145). Because of the photoinduced solid-to-liquid transitions of these polymers, light can to a certain degree heal cracks in azopolymers. Some azopolymers showed photoswitchable T_g and photoinduced solid-to-liquid transitions, but some others do not. Open questions are: why do polymers show photoswitchable T_g and photoinduced solid-to-liquid transition? How to design polymers with switchable T_g ? To answer these questions, we synthesize and characterize new model polymers.

Overview in Major Research Activities in Materials Engineering

by Folker H. Wittmann, Member EUAS

Short Biography

Folker H. Wittmann is born in Karlsruhe, Germany, April 20th 1936. He began to study physics and mathematics at Technische Hochschule Fridericiana (now Karlsruhe Institute of Technology, KIT) in Karlsruhe in 1955. After the first exams (Vordiplom) he changed 1958 to Ludwig Maximilian University Munich (LMU), where he finished his studies with a diploma in physics in 1961. He obtained his PhD from University of Technology in Munich (TUM) in 1964. Then he accepted the position of head of the Laboratory for Building Materials Physics at Munich University of Technology. He habilitated in Materials Physics in 1969.

He was nominated Professor for Building Materials Science at Delft University of Technology, The Netherlands, in 1976. Four years later, in 1980, he was nominated ordinary professor at École Polytechnique Fédérale de Lausanne (EPFL), Switzerland. In Lausanne he was professor for Building Materials Science and at the same time director of the materials testing laboratory at EPFL. Finally he was nominated ordinary professor for Materials Science at Swiss Federal Institute of Technology Zurich (ETHZ). He is professor emeritus since 2001.

As professor emeritus he continued teaching and his research at Qingdao University of Technology (QUT) in China.

Research Activities and Publications

His research activities can be subdivided into three major orientations: (1) Application of non-linear fracture mechanics to describe failure of composite materials, (2) Durability and service life of cement-based materials under combined mechanical and environmental loads, and (3) Physics of porous materials and their interaction with water.

He published until now more than 500 papers in leading scientific international journals and in proceedings of international conferences. Until today he edited more than 25 scientific volumes. For his research activities he obtained an honorary doctorate from University Duisburg-Essen in 1998. He is member of the editorial board of several international scientific journals. Between 1985 and 1987 he was president of the International Association for Structural Mechanics in Reactor Technology (IASMiRT) and between 1992 and 1995 he was president of the International Association for Fracture Mechanics in Concrete Structures (IAFRAMCOS). Between 1995 and 1997 he was president of International Union of Laboratories and Experts in Construction Materials (RILEM), later he was nominated honorary member of RILEM. He is also a member of the German Physical Society.

For his research and teaching activities at Qingdao University of Technology in China he was nominated honorary citizen of Shandong Province

Awards:

- 1976 RILEM Medal (Medaille Robert L'Hermite) for the fundamental research, which became the basis of the Munich Model to describe the interaction between hardened cement paste and water.
- 1985 Nomination Advisory Professor at Tongji University, Shanghai, China
- 1988 Fellow, American Ceramic Society
- 1988 Nomination Honorary Professor by Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
- 1991 Member of the Russian Academy of Sciences (АКАДЕМИЯ НАУК РСФСР)
- 1995 Honorary member of WTA, Association for science and technology in Restoration of Buildings and Protection of Monuments
- 1998 Honorary doctorate (Dr.-Ing. h.c.), in recognition of his outstanding performance in Science and Technology and for his pioneering work to strengthen interdisciplinary co-operation between scientists and civil engineers from Essen University, Department of Civil Engineering, Essen, Germany
- 2007 Qilu Award of Shandong Province, China, in recognition of remarkable achievements in research and teaching.
- 2008 Honorary member of RILEM, International Union of Laboratories and Experts in Construction Materials, Systems and Structures

- 2009 *Friendship Award, State Administration of Foreign Experts Affairs of the P. R. C.*
2010 *Fellow of IA-FraMCoS, International Association of Fracture Mechanics for Concrete and Concrete Structure*
2012 *The International Science and Technology Cooperation Award of the People's Republic of China*
2013 *Honorary citizen of Shandong Province, China*
2014 *Yuri Gagarin Medal in Gold from the Russian Academy of Architecture and Civil Engineering for introducing basic physical concepts into materials science*

My major research activities can be subdivided into four groups:

1. Fundamental aspects of creep and shrinkage of cement-based materials
2. Linear and non-linear Fracture Mechanics as applied to composite materials such as concrete
3. Strain-hardening fiber-reinforced cement-based composites, SHCC
4. Service-life, Durability, and sustainability of reinforced concrete structures

In the following essential results obtained shall be briefly presented.

1. Fundamental aspects of creep and Shrinkage of cement-based materials

During hydration of cement and hardening of fresh cement-based mixtures a nano-porous $\text{CaO}\cdot\text{SiO}_2\cdot\text{H}_2\text{O}$ (CSH) gel is formed. This gel is the matrix of hardening cement-based composites. The high internal surface of the hydration products, mainly calcium-silicate hydrates, which are covered with adsorbed cations, is in strong interaction with the surrounding water. At equilibrium moisture content with a surrounding atmosphere having a relative humidity below 50 % the surface of gel particles is covered by an adsorbed water film. This adsorbed water film reduces the surface energy of the gel particles. The surface energy of the hydration products depends on the thickness of the adsorbed water film. With decreasing thickness of the adsorbed water film the surface energy of the gel particles increases and hence the system is compressed. This process can be measured on a drying specimen as shrinkage. The reverse, i.e. swelling, is observed when the hydration products are rewetted. In equilibrium with a relative humidity of the surrounding air higher than 50 % disjoining pressure of the adsorbed water becomes big enough to separate hydration products which were in contact in the dry state. The disjoining pressure is responsible for shrinkage and swelling of cement-based materials in equilibrium with air having a relative humidity higher than 50 %. The change of surface energy and the action of disjoining pressure have also a strong influence on strength, elastic modulus, and creep of cement-based materials. The complex interaction between water and hydration products is well described by the Munich Model. This model is based on fundamental research of the influence of adsorbed water films on van der Waals interaction between two solid surfaces and on application of Mößbauer-effect to study the compression of nano-particles under the influence of surface tension.

Selected relevant publications:

- F. H. Wittmann, Grundlagen eines Modells zur Beschreibung charakteristischer Eigenschaften des Betons, Schriftenreihe Deutscher Ausschuss für Stahlbeton, Heft 290, pp.43-101 (1977)
F. Beltzung and F.H. Wittmann, Role of disjoining pressure in cement based materials, Cement and Concrete Research 35, 2364-2370 (2005)

2. Linear and non-linear Fracture Mechanics as applied to composite materials such as concrete

Strength of cement-based materials depends on duration of load and of size of specimens. Under high load cracks are formed in the composite structure of the material.

Crack formation in the composite structure of concrete was simulated by means of a powerful numerical model. If the applied load is high enough cracks will grow with time under load. This process has been described analytically by means of numerical models and results could be confirmed by extensive test series.

Strength of materials such as concrete depends considerably on the size of the specimens (size effect). To understand and describe this phenomenologically observed behavior local fracture energy was introduced. The local fracture energy varies with the width of the fracture process zone. As the crack approaches the back end of a specimen the fracture process zone becomes more and more confined and hence the local fracture energy decreases. Fracture energy in a concrete element is not a constant value. Theoretical predictions of this model were compared with relevant experimental results obtained with the wedge splitting technique, which was separately developed. It could be shown that a local variation of the fracture energy leads to a size dependence of the global specific fracture energy. On this basis the size dependent strength of concrete can be explained and predicted realistically.

Selected relevant publications:

F. H. Wittmann and J. Zaitsev, Verformung und Bruchvorgang poröser Baustoffe bei kurzzeitiger Belastung und Dauerlast, Deutscher Ausschuss für Stahlbeton, Heft 232, 65-145 (1974)

X.-Z. Hu and F. H. Wittmann, Fracture energy and fracture process zone, *Materials and Structures* 25, 319-326 (1992)

P. E. Roelfstra, Sadouki H., and Wittmann F. H., Le béton numérique, *Materials and Structures* 18, 327-335 (1985)

3. Strain-hardening fiber-reinforced cement-based composites, SHCC

Normal concrete may have high compressive strength but tensile strength remains rather limited. As a consequence drying shrinkage of young concrete exposed to natural environment with a relative humidity between 50 and 80 % leads in most cases to crack formation in the cover, which ought to protect steel reinforcement. Water and aggressive salts dissolved in water may penetrate rather quickly deep into reinforced concrete elements. But if chloride ions for instance reach the steel reinforcement, corrosion may start. Corrosion of steel in concrete is a major problem in all industrialized countries today. Repair of damaged steel reinforced concrete structures has become so expensive that necessary repair cannot be carried out in time because of the excessive cost (see section 4). In strain-hardening fiber-reinforced cement-based composites (SHCC) multiple fine cracks are formed instead of few wider cracks. Initially it was believed that water and salt solutions cannot penetrate these fine cracks. Detailed investigations have shown, however, that aggressive salt solutions may penetrate even fine cracks as formed in SHCC under load. There are two ways to improve durability of SHCC, however: (a) penetration of aqueous salt solutions can be avoided by surface impregnation with a water repellent agent such as silane and (b) self-healing of fine cracks by continuous hydration of remaining cement, or by filling the cracks with aqueous silicate solution, or by adding bacteria. By systematic research SHCC has become a promising material for more durable structures in the future.

Selected relevant publications:

F. H. Wittmann, Durability under Combined Loads, in G.P.A.G van Zijl and F. H. Wittmann (eds.), *Durability of Strain-Hardening Fibre-Reinforced Cement-Based*

Composites (SHCC), RILEM State of the Art Reports, Vol.4, Springer 2011.

F. H. Wittmann, Zhang P., and Zhao, T., Influence of combined environmental loads on durability of reinforced concrete structures, *Int. J. Restoration of Buildings and Monuments* 12, 349-370 (2006)

4. Service life, durability, and sustainability of reinforced concrete structures

All over Europe there are big bridges, which were built during the Roman Empire. Many of them survived 2000 years without major repair. Another example for longevity of concrete structures is the Pantheon in Rome, a concrete structure, which was built in seven years about 2000 years ago and which withstood earthquakes, wars and revolutions until today. Modern concrete bridges usually have to be repaired or even replaced after 50 years or less. About 12 % of the 607380 bridges in the US are rated as structurally deficient and the average service life is currently 44 years. The Federal Highway Administration (FHWA) estimates that to eliminate the nation's bridge deficient backlog by 2028, they would need to invest 20.5 billion \$ annually. This situation is similar or becomes similar in the near future in many countries. From this fact it becomes obvious that there is an urgent need to make reinforced concrete structures more durable.

Fracture energy and shrinkage induced crack formation in normal and high strength concrete was studied in detail. Surface impregnation of cracked concrete proved to be an effective method to avoid chloride penetration. It could be shown both in the laboratory and in practice that service life of steel reinforced concrete structures can be extended significantly by surface impregnation with water repellent agents or by surface protection with graphene. These protective methods have to be further developed in the near future.

Selected relevant publications:

F. H. Wittmann, Crack formation and fracture energy of normal and high strength concrete, *Sadhana (India)* 27 Part 4, 413-423 (2002)

F. H. Wittmann, H. Sadouki and A. Gerdes, Ionentransport und Beständigkeit zementgebundener Werkstoffe im Kontakt mit Wasser, *Int. J. Restoration of Buildings and Monuments* 6, 385-400 (2000)

F. H. Wittmann, P. Zhang and T. Zhao, Characteristics of the surface near water repellent layer, *Proc. 7th International Conference on Water Repellent Treatment and Protective Surface Technology for Building Materials, Hydrophobe VII*, pp. 11-18 (2014)

Recent Contributions in Solar Energy

by Antonio Lecuona-Neumann, Member EUAS

Short Biography

Antonio Lecuona-Neumann was born in 1953

Full professor in the Universidad Carlos III de Madrid (UC3M), Dep. of Thermal and Fluids Engineering.

Aeronautical Engineer in 1975 and PhD in 1980 with a Thesis on the numerical modelling of the compression with explosives of a micro-ball simulating the laser-driven nuclear fusion of D+T.

A few words can resume his research and teaching activity: Thermofluids and energy.

He has been continuously teaching subjects including: internal combustion engines, energy and environmental engineering, technical acoustics, turbomachinery, combustion, absorption machines, sources of energy and renewable energies, in several universities, either as nominal professor or invited at master and doctorate levels.

Invited Professor at Stanford University from 1986 to 87 in the HTGL laboratory.

He has acted as Vice-chancellor for Engineering studies, Director of Department and sub-director in the Engineering Schools of the Universities where he has being appointed.

Member of the Managing Commission for the establishment of the Universidad Carlos III de Madrid. For his contribution received the highest educational award in Spain "Encomienda de Alfonso X El Sabio"

Editorial board member of Applied Energy and Journal of Solar Energy. Currently, he acts as advisor for the Ministry of Science and Education of Spain as well as for other local governments and private organisations.

He has published two books in Spanish "Turbomáquinas" and "Cocinas Solares" and teaching material for 4 Open-Course-Ware courses in UC3M.

He has tutored 8 doctoral theses, 5 of them with extraordinary official prizes.

Member of the European Advisory Board in July 2005 and of the scientific board in 2006 of the "Centro de Tecnologías Avanzadas para la Combustión Limpia del Carbón" CIEMAT, Spain. This task group was oriented to research in CO₂ capture in Spain.

He has contributed to about 100 talks and conferences to national and international congresses.

Author and co-author of 10 national patents.

He is co-author of more than 50 ISI registered papers with "h" factor above 20. Around 1.400 cites.

He has participated in 8 European Commission competitive research projects PIVNET, PIVNET2, EUROPIV, EUROPIV2, LSP, LOWNOXIII, COJEN and HOT, as well as in many industrial projects.

FULLY INTEGRATED SOLAR THERMAL ENERGY

Currently, the production of solar heat is carried out using a Heat Transfer Fluid (HTF) that transports the heat from a solar collector to consumption through a heat exchanger. The HTF has to withstand both high temperatures and ones below freezing point, excepting the case of large power plants. This makes necessary to use synthetic oils or water with anti-freezing additives. Both are expensive, short lived, polluting and above this, oils pose fire risks. Industrial and building solar acclimatisation applications are idle because of the complexity and cost that this implies. But this is not the single barrier.

Let's assume that solar heat production is of paramount importance for industrial processes, not only for its direct application but also for converting it into cold using absorption machines. A sustainable society needs to use solar energy and thermal applications in huge amounts, for heating, preserving, freezing, acclimatising,

dehumidifying and in addition to that for power production by thermo-solar plants. Energy resilience needs local production and full integration with different energy sources either for injecting energy for others or for consuming it when necessary.

This brings the idea of machines using advanced absorption technology with direct vapour production. These machines were historically the first ones to produce cold, and even a young Albert Einstein devoted 9 years investigating on them. They consume heat instead of electricity and they are nowadays less competitive than the more compact and cheaper mechanical compression machines. Low to medium temperature (MT) heat is easily produced by solar thermal collectors with a higher efficiency than photovoltaic (PV) panels.

An absorption machine can be configured to amplify the solar heat (heat pump or heat converter), produce cold and even produce power when neither heat nor cold is demanded by the user. Recent own investigations have demonstrated that when solar is insufficient, the hybrid absorption cycles can consume grid electricity to satisfy the user demand. This way advanced absorption machines can represent the backbone of a very flexible and integrated energy system for buildings and industries, consuming solar thermal energy and minimising the need for energy storage.

Back to the troubling HTFs, the ongoing research focuses on eliminating them. The working fluid of the absorption machine is proposed to be drawn directly into the solar collector. The installation will be much simplified. The working fluid is based on a natural much-produced and used refrigerant, NH_3 and a recyclable salt LiNO_3 . No greenhouse neither ozone depleting effects are involved when escaping. Full outdoor installation is possible, avoiding the use of valuable floor indoors.

Theoretical models show good perspectives and initial experimentation support the model's results. The development of industrial prototypes is expected in the following years.

CLEAN SOLAR COOKING FOR ALL

According to many sources, there are from 2 to 4 million worldwide premature deaths attributed to indoor air pollution caused by burning for cooking and heating inside dwellings. Firewood, dung and agriculture residues (biomass) are burned in very low-efficiency cookstoves for cooking and eventually simultaneous space heating, sanitary hot water production and sterilisation, especially in the developing world. This happens for about 2 billion people. Fumes exhaust is typically non-effective and sometimes undesired by ignorance. Mainly flying particles cause cancers, pulmonary and circulatory diseases. Consumption of firewood causes deforestation and collection takes a long time for women and children on daily basis. Also, some non-negligible global warming and is caused by deforestation as well as external atmospheric pollution.

Improved cookstoves have been deployed in developing countries trying to help to reduce this problem, but it is still there.

A non-recent solution is possible, **solar cooking**. This way just exposing to the sunshine a solar (thermal) cooker with a black pot containing the food, after some time full cooking is performed. Many barriers difficult its acceptance and widespread use. Improved types of solar cookers are periodically introduced and in-situ tested. But substantive steps forward toward full implementation are not evident nowadays.

One problem to solve is cooking with no sun. Thus energy storage is needed as well as a backup. Owing to the high cost of producing a fuel (e. g. H_2) as a storage medium or of using costly batteries, the development of a Thermal Energy Storage (TES) has been endeavoured by the research group I lead.

A Phase Change Material (PCM) has been found to be ideal; cheap, edible and with a high latent heat of fusion. It is erythritol, a sugar alcohol much used as non-caloric sugar. It melts at 118 °C storing 340 kJ/kg, similar to ice. When solidifying it can boil water if a heat conductivity enhancer is inserted.

A pot containing this material can be melted (charged) during the day and stored in a well-insulated container (e. g. locally manufactured hay basket) so that cooking the dinner and the following day breakfast is possible for a family with a utensil weighing less than 10 kg. With this apparatus cooking outdoors still is necessary, what is an inconvenience, especially in peri-urban areas.

In parallel, there is a move toward deploying very small PV solar panels, around 25 Wp, to provide families with charging capacity for their mobiles, as a tool for development. The menacing home fire is still there every day.

A larger PV panel, in the order of 2 m² cost nowadays 300 € at retail prices, with the potential to halve this price at a large market scale. A family with it installed on the roof can cook and store the heat for dinner and breakfast with a PCM based device that can cost 50 €, materialising the **PV solar cooker**. This device is based on a commercial cooking robot fed with 230 V AC that includes thermal insulation. It must be modified with an added resistance capable of dissipating the PV panel 24 V DC power. A new type of electronic controller for this setup is necessary as there is no battery, the most costly and difficult to transport element that has been eliminated. This controller is under development with the aim that it can be constructed and maintained locally with a cost lower than 20 €. The cooking robot can still be used when the grid reaches the developing family dwelling.

Availability of the 300 Wp PV panel system by these poor families will enter them in a plethora of modern possibilities, such as charging small consumption devices, like mobiles, tablets, radios, TVs, etc., as well as empowering them to self-sufficiency and sustainability. Expansion of this basic energy resource will allow powering fans, refrigerators and what else is demanded.

Numerical modelling and laboratory experiments have been performed on this idea with promising results. In-situ trials are foreseen.

Schools, hospitals and public facilities can benefit from this proposal, this way educating children toward the non-intuitive use of the sun for a very basic need: clean cooking.

A recent international project (AESCA) within the Hispanic community has addressed the topic of energy supply to isolated communities, financed by CYTED.

FLOW MODELLING AND DIAGNOSTIC TECHNIQUES

Advanced Particle Image Velocimetry techniques have been developed (LFC-PIV) as well as an optical non-intrusive technique for spray characterization, able to remotely measure size, shape, velocity and number of droplets.

The knowledge gained on disperse two-phase flows in a previous research project and on turbomachinery has allowed winning in an open call the responsibility of developing the project “HUMIDITY OPTIMIZATION TOOL (HOT)” within the Clean Sky European Commission program. In this project, the problem of **fog formation** in the cabin of aircraft was analysed, measured and a model developed to predict and avoid its appearance.

Development of Green Cements and Sustainable Infrastructure

by Paulo Monteiro, Member EUAS

Short Biography

Professor Monteiro is the Roy W. Carlson Distinguished Professor at the Department of Civil and Environmental Engineering, University of California, Berkeley. He is at the forefront of developing strategies to improve the long-term performance of concrete structures. The first to develop soft X-ray spectromicroscopy using synchrotron radiation to image chemical reactions in real time, he modernized the study of hydration mechanism. Professor Monteiro's achievements in experimental research include: (1) pioneering the use of low-temperature scanning electron microscopy to image ice formation in porous cement paste; (2) developing total scattering methods to study calcium silicate hydrates in order to optimize its nanostructure; (3) creating the first high-resolution nanotomography of hydration products using X-rays; and (4) engineering a comprehensive nanostructure characterization of ancient Roman concrete to unlock the secret of its durability. His contributions also include developing rigorous mathematical theories to model material behavior, such as: analysis of interphases in concrete, modeling cryo-suction of concrete exposed to freezing temperatures using poromechanics, scaling laws for durability predictions, and fluid flow in nano-porous media. He has published over 240 archival papers and co-authored with P.K. Mehta the classical textbook, Concrete: Microstructure, Properties, and Materials, 4th edition, McGraw Hill, (2014), which has been translated to Japanese, Chinese, Greek, Spanish, Portuguese, and Persian.

His has received the following awards for his research: Outstanding Paper Award, International Conference on Sustainable Construction Materials and Technologies, Kyoto, Japan; Honra ao Merito Award from IBRACON; Premio Ari Torres, highest award for concrete research given by the Brazilian Concrete Institute; Brunauer Award from the American Ceramics Society; Wason Medal for Materials Research, from the American Concrete Institute; Livre Docente from the University of São Paulo, Brazil; and the Presidential Young Investigator Award from the U.S. National Science Foundation.

Concrete is the largest manufactured product used today. On average, concrete mixtures for general construction are composed of 12% Portland cement (PC), 8% mixing water, and 80% coarse and fine aggregate by mass. In 2014, the global concrete industry consumed nearly 4.2 billion tonnes Portland-cement clinker and 28 billion tonnes of aggregate, in addition to 2.8 billion tonnes of mixing water and small amounts of chemical admixtures. The mining, processing, and transport of such huge quantities of materials for the production of concrete, in addition to large amounts of limestone, clay, and fossil fuels for PC clinker manufacture, require considerable energy and adversely affect the ecology of virgin lands.

Portland cement is a manufactured product that is the principal hydraulic binder used in modern concrete mixtures; it is not only energy-intensive (4 GJ/tonne of cement) but also responsible for large emissions of CO₂. The manufacture of 1 tonne of PC clinker releases 0.8 to 1 tonne CO₂ into the atmosphere. The world's yearly cement production of 4.2 billion tonnes of mostly PC is responsible for nearly 7% of the total global CO₂ emissions. In the United States, cement and concrete production is a \$50 billion industry. In addition, the construction industry generates \$650 billion/year and employs 7 million people.

Unfortunately, America's infrastructure was built mostly during the 1940s and is now aging and needs to be replaced. This widespread crisis threatens public safety, industrial development, and

economic growth. On March 19, 2013, the American Society for Civil Engineers (ASCE) released its fifth *Report Card for America's Infrastructure*. Conducted by an Advisory Panel composed of the nation's leading civil engineers whose areas of expertise cover a broad spectrum, ASCE conferred an overall grade of "D+" and estimated that an investment of 3.6 trillion U.S. dollars will be needed to raise the grade to a "B" level by 2020.

The microstructure and properties of concrete can be altered by cost-effective methods that improve the impermeability and durability on exposure to weather extremes. At present, most of the feasible options for microstructural improvement have already been implemented. Thus, there is an urgent need to find scientific and technically-viable improvements in the atomic and nanostructure of the cementitious phases to increase concrete strength and durability. Such improvements will reduce the cement content in a concrete mixture and, therefore, its carbon footprint. Optimizing the properties of Portland cement, concrete's principal binding phase, calcium silicate hydrate (C-S-H), is a potential strategy to achieve concrete with better performance and more durability while still reducing its carbon footprint. Calcium silicate hydrate exists as a solid solution with variable structure and chemical composition, and can coexist with other solid phases at thermodynamic equilibrium. It is also poorly crystalline and hierarchically porous at multiple length scales. Such characteristics make it exceedingly difficult to probe composition-structure-property correlations of pore-free C-S-H. Calcium aluminosilicate hydrate (C-A-S-H) can be formed when supplementary cementitious materials (SCMs), such as fly ash, blast-furnace slag, and volcanic ash, containing aluminum. Calcium aluminosilicate hydrate synthesized hydrothermally at room temperature lacks long-range crystallinity but has an atomic structure analogous to tobermorite, i.e., stacked layered structures (along the *c*-axis), with aluminosilicate dreierketten chains clamping on either side of CaO_7 double sheets, with zeolitic water and charge-balancing ions (e.g., Ca^{2+}) in the interlayer space (see **Figure 1a**). Every two-paired-site $\text{Si}(\text{Al})\text{O}_4$ tetrahedra are connected by a bridging site tetrahedron in the dreierketten chain structure, which runs parallel to the *b*-axis. The intralayer and interlayer, as separated by the bridging Si site, together lead to basal spacings of $\sim 9\text{--}16$ Å in the C-(A)-S-H structure. Unlike macro-crystalline tobermorite, C-(A)-S-H is often nano-crystalline and contains defects such as vacancies and Si for Al substitution in bridging sites. It can also accommodate a range of water molecules and aqueous species (e.g., Ca^{2+}) in the interlayer space, and cross-linking of adjacent dreierketten chains can occur; see **Figure 1b**.

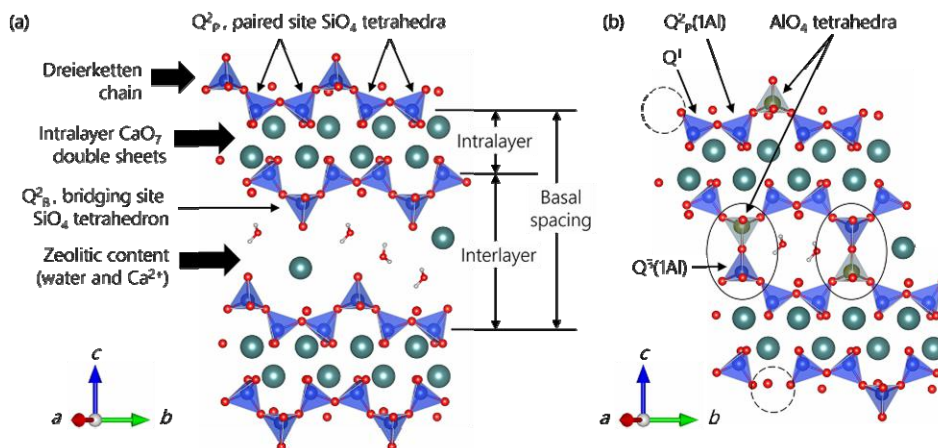


Figure 1. Schematics of (a) crystalline C-S-H (modified from 14 Å tobermorite) and (b) C-A-S-H atomic structures with Al-induced cross-linking (solid circles). Spheres of blue, red, green, white, and yellow colors represent Si, O, Ca, H and Al, respectively; and (b) the dashed circles are tetrahedral Si vacancies in bridging sites. The conventional $Q^n(m\text{Al})$ -notation is used, which describes aluminosilicate chain polymerization, e.g., Si tetrahedra are connected to *n* adjacent tetrahedra (SiO_4 or AlO_4), of which *m* are AlO_4 ; subscripts P and B represent paired and bridging sites, respectively (after Myers *et al.*, 2015, *Cem. Concr. Res.*, 68, 83–93).

Recently our research group has been involved in the following paradigm shifts:

(1) *Densification of the interlayer spacing governs the nano-mechanical properties of calcium-silicate-hydrate (C-S-H)*

We used synchrotron radiation-based high-pressure X-ray diffraction to quantify the influence of dreierketten chain cross linking on the anisotropic mechanical behavior of C-(A-)S-H. We demonstrated that the ab-planar stiffness is independent of dreierketten chain defects, e.g. vacancies in bridging tetrahedra sites and Al for Si substitution; see Figure 2. The c-axis of non-cross-linked C-(A-)S-H is more deformable due to the softer interlayer opening but stiffens with decreased spacing and/or increased zeolitic water and Ca^{2+} of the interlayer. Dreierketten chain cross links act as ‘columns’ to resist compression, thus increasing the bulk modulus of C-(A-)S-H. We provided the first experimental evidence on the influence of the Al-induced atomistic configurational change on the mechanical properties of C-(A-)S-H.

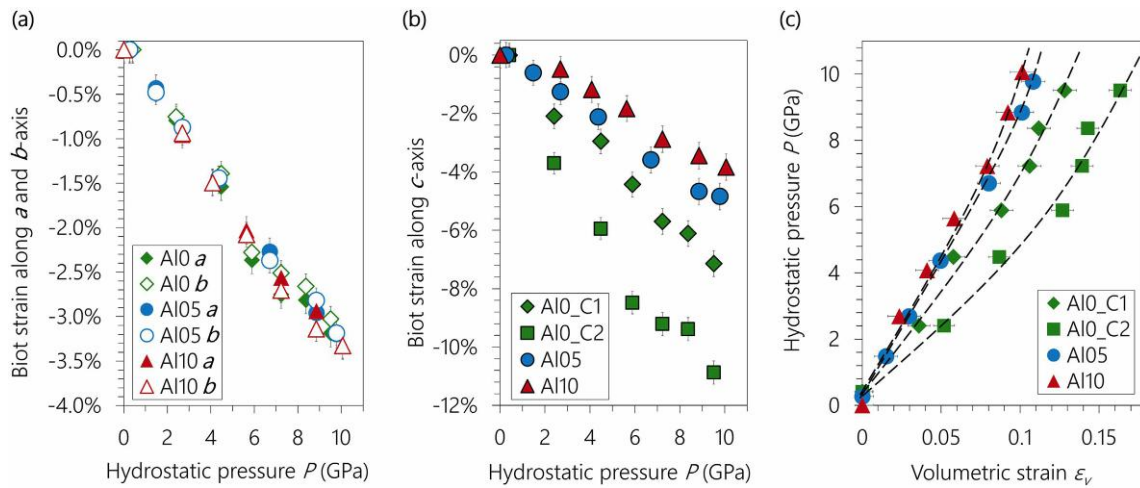


Figure 2. Biot strains as functions of applied hydrostatic pressure along (a) a- and b-axes, (b) c-axis, and (c) hydrostatic pressure as a function of volumetric strain. Biot strain is defined as $\epsilon = L/L_0 - 1$, where L and L_0 are the current and initial length of unit cell edge, respectively. The error bars of the axial Biot strains and the volumetric strain originate from the refinement uncertainties. The uncertainty of pressure is estimated to be ~ 0.15 GPa. Dashed curves in (c) illustrate the fitted results of BM-EoS. Notation: Al0, Al5 and Al10 correspond to C-A-S-H containing 0, 5, and 10% of Al. (Geng et al., *Scientific Reports*, 2017)

(2) *Morphological quantification of hierarchical calcium silicate hydrates by X-ray nano-CT bridges the gap from nano- to micro-length scales*

To investigate the porous structure of materials, various techniques, including transmission electron microscopy (TEM), scanning electron microscopy, and X-ray micro-tomography have been used. Despite these advances, only a few techniques allow in situ and undisturbed higher resolution 3D imaging for length scales ranging between a few tens of nanometers to several hundreds of nanometers. Recent resolution advances in soft X-ray transmission microscopy offer unique opportunities for exploring materials at this length scale. Transmission X-ray microscopy (TXM) is a versatile, non-invasive technique for imaging samples with a thickness well above that used for a TEM sample and even allows imaging of samples in aqueous solution, thereby preventing the generation of drying artifacts.

Using limited angle nano-tomography from TXM transmission images, our team obtained the first

high-resolution 3D images of hydrated cement paste¹. Although a single 2D transmission image is not sufficient to get a 3D representation of a complex pore network, the one-frame-per-second investigation of the sample is perfectly adequate for kinetic studies. Based on the Fourier slice theorem, it is possible to compute ultra-small angle-scattering patterns; however, it remains a challenging experiment that is largely used to characterize geomaterials. The technique has become much more powerful with the advent of soft X-ray ptychography, which uses coherent diffraction patterns and allows a high spatial-resolution morphology. Our research group reported the first use of high-resolution soft X-ray ptychography image of C-S-H and morphological quantification of C-S-H, to distinguish the contributions of C-S-H forming inside the original cement grain and the C-S-H formed in the space between grains to the small angle scattering of cement paste (see Figure 3). This line of research may provide unique information on the meso-structure of the cementitious matrix in concrete.

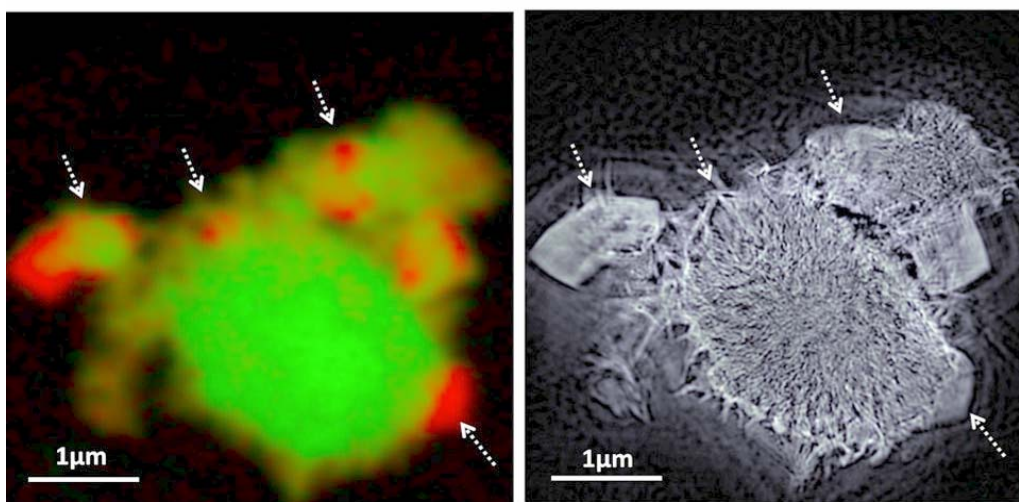


Figure 3. Traditional Scanning Transmission X-ray micrograph (left) and a soft X-ray ptychographic image (right) of 17 d hydrated cement grain. The soft X-ray ptychographic was able to image the individual fibers of C-S-H (from Bae *et al.*, 2015, *J. Am. Ceramic Soc.*, doi:[10.1111/jace.13808](https://doi.org/10.1111/jace.13808))

(3) *Unlocking the mechanical resilience and cementitious processes in Imperial Roman architectural mortar*

The pyroclastic aggregate concrete of Trajan's Markets (110 CE) has absorbed energy from seismic ground shaking and long-term foundation settlement for nearly two millennia while remaining largely intact at the structural scale. We recently reported² the scientific basis of this exceptional service record through computed tomography of fracture surfaces and synchrotron X-ray microdiffraction analyses of a reproduction of the standardized hydrated lime–volcanic ash mortar that binds decimeter-sized tuff and brick aggregate in the conglomeratic concrete. We identified that platey strätlingite crystals toughen interfacial zones along scoria perimeters and impede macroscale propagation of crack segments. In the 1,900-y-old mortar, C-A-S-H has low $\text{Ca}/(\text{Si}+\text{Al}) \approx 0.45\text{--}0.75$. Dense clusters of 2- to 30- μm strätlingite plates further reinforce interfacial zones, the weakest link of modern cement-based concrete, and the cementitious matrix.

¹ S. Brisard *et al.*, *Am. Mineralogist*, 97, 2–3 480–483, FEB-MAR 2012.

² M. D. Jackson, (2014). *PNAS* 111(52), 18484–18489. doi:[10.1073/pnas.1417456111](https://doi.org/10.1073/pnas.1417456111)

New Contributions in Airway Disease Research

by Peter Barnes, Member EUAS

Short Biography

Airway Disease Section, National Heart and Lung Institute, Dovehouse St, London SW3 6LY

Education:

1966-69 Preclinical: Cambridge University (St Catharine's College)(Double first degree)
Open Scholarship, elected to title of Scholar

1969-72 Clinical: Oxford University Medical School (Clinical Scholarship)

Previous appointments:

1975-1978: Registrar (General Medical Rotation), University College Hospital, London

1978-1979: MRC Research Fellow and Honorary Senior Registrar, Dept of Clinical Pharmacology,
Royal Postgraduate Medical School, London

1979-1982 Senior Registrar (Resp Medicine) Hammersmith Hospital, London

1981-1982 MRC Travelling Fellowship to CVRI, University of California

1982-1985 Consultant Physician, Hammersmith Hospital, London

1985-1987 Professor of Clinical Pharmacology, Cardiothoracic Institute

Current Appointment (since 1987): funded by HEFCE

Margaret-Turner-Warwick Professor of Thoracic Medicine, National Heart & Lung Institute

Head of Respiratory Medicine, Imperial College

Honorary Consultant Physician, Royal Brompton Hospital

Degrees, Honours and Awards

1982 DM: Oxford University (Thesis: Adrenergic mechanisms in asthma)

1986 FRCP: Royal College of Physicians

1987 DSc: Oxford University

1990 Linacre Lecture, Royal College of Physicians, London

1994 Goldberg Prize, University of Chicago

1996 Amberson Lecture, American Thoracic Society (most prestigious lecture)

1997 Honorary MD, University of Ferrara, Italy

1998 Fellow Academy of Medical Sciences (FMed Sci, Founding Fellow)

1999 Sadoul Lecture, European Respiratory Society (most prestigious lecture)

2000 Honorary MD, University of Athens, Greece

2005 Honorary MD, University of Tampere, Finland

2007 Fellow of Royal Society (first respiratory scientist for >150 years)

2007 Presidential Award, European Respiratory Society

2008 British Thoracic Society Gold Medal

2009 NIHR Senior Investigator

2009 Croonian Lecture, Royal College of Physicians, London

2010 Honorary MD, Leuven University, Belgium

2011 Honorary Fellow of St Catharine's College, Cambridge

2012 Member of Academia Europaea (Academy of Europe, MAE)

Master Fellow, American College of Chest Physicians (one of only 2 outside N America)

2013-2014 President of European Respiratory Society (largest respiratory society in the world)

2014 Honorary degree, Maastricht University, Holland

Elected Member of Association of American Physicians

Wellcome Lecture, Royal Society of Medicine (most prestigious lecture)

2015 Galen Medal, Society of Apothecaries, London (most prestigious award)

President's Award for Scientific Innovation, Imperial College

Research

My research concerns the cellular and molecular mechanisms of inflammation in asthma and COPD and identification of novel therapeutic targets in these diseases. I research the aberrant immune and signalling pathways in severe asthma and COPD.

Recent research funding

- Wellcome Trust (Program Grant) "Oxidative stress-induced inflammatory gene expression and ageing in COPD: role of sirtuin-1 and histone methylation. £976 (2011-2016)
- MRC-ABPI COPD Consortium: "The mechanisms, impact and therapeutic targeting of bacterial colonization of the airways in COPD" £6,000k (2011-2015) [PI]
- MRC-Indian Medical Research Council: "Phenotypic characterisation of non-smoking COPD" £646k (2012-2015)[PI]
- Pfizer. "Treating inflammation, remodelling and defective phagocytosis in COPD" £2,200k (2013-2016) [PI]
- NIHR HTA. "A randomised, double-blind placebo controlled trial of the effectiveness of low dose oral theophylline as an adjunct to inhaled corticosteroids in preventing exacerbations of chronic obstructive pulmonary disease" £2,118k (2013-2015) [Coapplicant]

University Spin-out Company

Co-founder of RespiVert, an Imperial College spin-out company established to find novel inhaled drugs for the treatment of corticosteroid-resistant lung inflammation in COPD and severe asthma. After the discovery of several novel compounds, the company has been sold to Johnson & Johnson, who are now conducting Phase 2 and 3 trials in severe asthma and COPD patients.

Editorial

Associate Editor: *Am J Respir Crit Care Med* (1999-2004; 2010-14); *Chest* (2003-now), *PLoS Medicine: Respiratory Editor* (2004-now); *Founding Editor: Pulmonary Pharmacology, Respiratory Research*; *Editor: Up-to-Date - Pulmonary Medicine*. Editorial boards: *New Engl J Med* (1994-2005) + 30 other journals

Publications

Over 1000 peer reviewed publications. Most highly cited respiratory researcher in the world and most highly cited clinical researcher in Europe over last 25 years (*h-index* = 156, >120,000 citations)

17th most highly cited scientist ever in the world. Author and editor of over 50 books on airway disease and pharmacology.

I am an international leader in airway disease research, the most highly cited respiratory researcher in the world over the last 30 years (ISI), and have authored the most influential articles in COPD (*Int J COPD* 2015). My research has focussed on understanding underlying inflammatory mechanisms and therapies for airway diseases. I have published >1200 peer reviewed articles and have an *h-index* of 156 with >120,000 citations. I was elected FRS in 2007, the first respiratory researcher for >150 years.

My research into the inflammatory mechanisms in asthma, understanding the role of proinflammatory transcription factors and the molecular mechanisms whereby corticosteroids suppress this inflammation were important in promoting the use of inhaled corticosteroids to control all patients with persistent asthma symptoms, revolutionising the management of asthma. I have explored the molecular interactions of β_2 -agonists and corticosteroids, providing a scientific rationale for the use of steroid-LABA combination inhalers. My research group pioneered the use of exhaled biomarkers, particularly nitric oxide, to monitor inflammation in asthma leading to the use of exhaled NO in clinical practice.

My group discovered the long duration of the muscarinic receptor antagonists tiotropium and glycopyrrolate, which are now used as the bronchodilators of choice in COPD. My group showed that the poor response to corticosteroids in patients with COPD and severe asthma is explained by reduced activity and expression of HDAC2, which is secondary to oxidative stress through activation of PI3K- δ . Theophylline reverses steroid resistance by increasing HDAC2 activity via directly inhibiting this enzyme. Other existing drugs, including tricyclic antidepressants and macrolides, also interact inhibit this pathway to reverse corticosteroid resistance. I am a co-founder of a spin-out company, RespiVert, which developed novel potent inhaled drugs to treat steroid-resistant inflammation and now entering phase 2 studies in severe asthma and COPD.

Key publications

1. Mitani A, Ito K, Vuppusetty C, Barnes PJ, Mercado N. Inhibition of mTOR restores corticosteroid sensitivity in chronic obstructive pulmonary disease. *Am J Respir Crit Care Med* 2015; 193:143-53. PMID:26426522.
This study demonstrates PI3K and mTOR activation in COPD and a new and additional mechanism of corticosteroid resistance involving c-Jun and AP-1 activation, in addition of reduced HDAC2 activity.
2. Wiegman CH, Michaeloudes C, Haji G, Narang P, Clarke CJ, Russell KE, Bao W, Pavlidis S, Barnes PJ, Kanerva J, Bittner A, Rao N, Murphy MP, Kirkham PA, Chung KF, Adcock IM.
Oxidative stress-induced mitochondrial dysfunction drives inflammation and airway smooth muscle remodeling in patients with chronic obstructive pulmonary disease. *J Allergy Clin Immunol* 2015; 136:769-80. PMID: 25828268.
3. Maneechotesuwan K, Wongkajornsil A, Adcock IM, Barnes PJ. Simvastatin suppresses airway IL-17 and up-regulates IL-10 in patients with stable COPD. *Chest* 2015; 148:1164-76. PMID:26043025.
4. Michaeloudes C, Mercado N, Clarke C, Bhavsar PK, Adcock IM, Barnes PJ, Chung KF. Bromodomain and extraterminal proteins suppress NF-E2-related factor 2-mediated antioxidant gene expression. *J Immunol* 2014; 192: 4913-20. PMC4011694.
5. Chana KK, Fenwick PS, Nicholson AG, Barnes PJ, Donnelly LE. Identification of a distinct glucocorticosteroid-insensitive pulmonary macrophage phenotype in patients with chronic obstructive pulmonary disease. *J Allergy Clin Immunol* 2014; 133: 207-16. PMID:24176116
6. Mercado N, Kizawa Y, Ueda K, Xiong Y, Kimura G, Moses A, Curtis JM, Ito K, Barnes PJ. Activation of transcription factor Nrf2 signalling by the sphingosine kinase inhibitor SKI-II is mediated by the formation of Keap1 dimers. *PloS one* 2014; 9: e88168. PMC3914928.
7. Hakim A, Barnes PJ, Adcock IM, Usmani OS. Importin-7 mediates glucocorticoid receptor nuclear import and is impaired by oxidative stress, leading to glucocorticoid insensitivity. *FASEB J* 2013; 27: 4510-9.
8. Haque R, Hakim A, Moodley T, Torrego A, Essilfie-Quaye S, Jazrawi E, Johnson M, Barnes PJ, Adcock IM, Usmani OS. Inhaled long-acting β 2-agonists enhance glucocorticoid receptor nuclear translocation and efficacy in sputum macrophages in COPD. *J Allergy Clin Immunol* 2013; 132: 1166-73. PMID:24070494.
9. Paschalaki KE, Starke RD, Hu Y, Mercado N, Margariti A, Gorgoulis VG, Randi AM, Barnes PJ. Dysfunction of endothelial progenitor cells from smokers and COPD patients due to increased DNA damage and senescence. *Stem Cells* 2013; 31: 2813-26. PMC4377082.
This study demonstrates for the first time that endothelial precursor cells from COPD patients show cellular senescence and DNA damage and have a reduced capacity to repair

damaged vascular endothelium. This provides a mechanism that links ageing of lungs and cardiovascular systems in COPD patients accounting for the high prevalence of cardiovascular disease in COPD patients.

10. Mercado N, Thimmulappa R, Thomas CM, Fenwick PS, Chana KK, Donnelly LE, Biswal S, Ito K, Barnes PJ. Decreased histone deacetylase 2 impairs Nrf2 activation by oxidative stress. *Biochem Biophys Res Commun* 2011; 406: 292-8. PMC3061319.

We showed that there is a reduced Nrf2 response to oxidative stress in COPD compared to the normal response seen in normal smokers. This is related to acetylation of Nrf2 as a result of the decreased HDAC2 activity in COPD. Acetylated Nrf2 has reduced efficacy for activating antioxidant genes.

11. Maneechotesuwan K, Yao X, Ito K, Jazrawi E, Usmani OS, Adcock IM, Barnes PJ. Upregulation of GATA-3 nuclear import and phosphorylation: a novel mechanism of corticosteroid action in allergic disease. *PLoS Med* 2009; 6: e1000076. PMID:19436703

This study showed that corticosteroids are highly effective against allergic inflammation that is driven by GATA3 through competition between GATA3 and glucocorticoid receptors entering the nucleus via a common nuclear import protein importin- α , as well as via increased expression of MKP-1 which inhibits p38 MAP kinase, that is necessary for GATA3 nuclear translocation.

12. Nakamaru Y, Vuppusetty C, Wada H, Milne JC, Ito M, Rossios C, Elliot M, Hogg J, Kharitonov S, Goto H, Bemis JE, Elliott P, Barnes PJ, Ito K. A protein deacetylase SIRT1 is a negative regulator of metalloproteinase-9. *FASEB J* 2009; 23: 2810-19. PMID:19376817.

We showed that reduced sirtuin-1 expression and activity in COPD lung as a result of oxidative stress and that this resulted in increased expression of the elastase MMP9. In mice exposed to cigarette smoke the decreased sirtuin-1 and increased MMP9 were restored to normal by a novel sirtuin-activating compound SR2271.

13. To Y, Ito K, Kizawa Y, Failla M, Ito M, Kusama T, Elliot M, Hogg JC, Adcock IM, Barnes PJ. Targeting phosphoinositide-3-kinase- δ with theophylline reverses corticosteroid insensitivity in COPD. *Am J Resp Crit Care Med* 2010; 182: 897-904. PMID:20224070.

We demonstrated that oxidative stress activates PI3K δ , resulting in phosphorylation and reduced activity and expression of HDAC2. This is reversed by a low concentration of theophylline, which selectively inhibits oxidant-activated PI3K δ and thus is able to reverse corticosteroid resistance induced by oxidative stress.

14. Ito K, Yamamura S, Essilfie-Quaye S, Cosio B, Ito M, Barnes PJ, Adcock IM. Histone deacetylase 2-mediated deacetylation of the glucocorticoid receptor enables NF- κ B suppression. *J Exp Med* 2006; 203: 7-13. PMID:16380507.

For the first time we showed that acetylation of the glucocorticoid receptor as a result of reduced HDAC2 activity regulates its functional effect with reduced trans-repression of inflammatory genes but no effect on trans-activation of genes. This mechanism explains how reduced HDAC2 activity causes corticosteroid resistance.

15. Ito K, Ito M, Elliott WM, Cosio B, Caramori G, Kon OM, Barczyk A, Hayashi M, Adcock IM, Hogg JC, Barnes PJ. Decreased histone deacetylase activity in chronic obstructive pulmonary disease. *N Engl J Med* 2005; 352: 1967-76. PMID:15888697.

For the first time we showed that acetylation of the glucocorticoid receptor as a result of reduced HDAC2 activity regulates its functional effect with reduced trans-repression of inflammatory genes but no effect on trans-activation of genes. This mechanism explains how reduced HDAC2 activity causes corticosteroid resistance but side effects are unaffected.

16. Cosio BG, Tsaprouni L, Ito K, Jazrawi E, Adcock IM, Barnes PJ. Theophylline restores histone deacetylase activity and steroid responses in COPD macrophages. *J Exp Med* 2004; 200: 689-695. PMID:15337792.

This study showed that low doses of theophylline are able to reverse corticosteroid resistance in airway epithelial cells of COPD patients by restoring HDAC2 activity and expression to normal levels and that this effect is prevented by an HDAC inhibitor trichostatin A.

17. Ito K, Lim S, Caramori G, Cosio B, Chung KF, Adcock IM, Barnes PJ. A molecular mechanism of action of theophylline: Induction of histone deacetylase activity to decrease inflammatory gene expression. *Proc Natl Acad Sci USA* 2002; 99: 8921-6. PMID:12070353.

18. Ito K, Barnes PJ, Adcock IM. Glucocorticoid receptor recruitment of histone deacetylase 2 inhibits IL-1 β -induced histone H4 acetylation on lysines 8 and 12. *Mol Cell Biol* 2000; 20: 6891-903. PMID:10958685.

This study is the first demonstration that glucocorticoids signal through epigenetic mechanisms and trans-activate genes via histone acetylation by histone acetyltransferase activation and suppress inflammatory genes at low concentrations through recruitment of HDAC2 and activated glucocorticoid receptor to the activated inflammatory gene complex which is associated with acetylation of histone-4.

19. Leckie MJ, ten Brincke A, Khan J, Diamant Z, O'Connor BJ, Walls CM, Mathur M, Cowley H, Chung KF, Djukanovic RJ, Hansel TT, Holgate ST, Sterk PJ, Barnes PJ. Effects of an interleukin-5 blocking monoclonal antibody on eosinophils, airway hyperresponsiveness and the late asthmatic response. *Lancet* 2000; 356: 2144-8. PMID:11191542.

20. Kharitonov SA, Yates D, Robbins RA, Logan-Sinclair R, Shinebourne E, Barnes PJ. Increased nitric oxide in exhaled air of asthmatic patients. *Lancet* 1994; 343: 133-5. PMID:7904001.

This was the first study that showed that fractional exhaled nitric oxide (FENO) is related to airway inflammation in asthma patients and is reduced by anti-inflammatory therapy with corticosteroids. FENO measurements are now used to monitor asthma control in clinical practice and to monitor corticosteroid adherence.

Materials Science, Fracture Mechanics & Fatigue-Crack Propagation

by Robert Ritchie, Member EUAS

Short Biography

Robert O. Ritchie is the H.T. & Jessie Chua Distinguished Professor of Engineering at the University of California, Berkeley, and Senior Faculty Scientist at the Lawrence Berkeley National Laboratory. He received M.A., Ph.D. and Sc.D. degrees in Physics/Materials Science from Cambridge University.

He is known for his research into the mechanics and micro-mechanisms of fracture and fatigue of a broad range of structural and biological materials, where he provided a microstructural basis for their damage-tolerance and fatigue resistance. He has published over 700 papers and edited 19 books in the technical literature, with an h-index of 101 (Google Scholar). Currently, his interests are focused on high-entropy and bulk-metallic glass metallic alloys, the structural integrity of human bone, and the development of novel structural materials inspired by Nature.

He has won numerous awards, recently the Turnbull Award from the Materials Research Society (2013), the Acta Materialia Gold Medal (2014), and the TMS Morris Cohen Award (2017); he was also the inaugural winner of the Sir Alan Cottrell Gold Medal from the International Congress on Fracture (2009). In addition to the EUAS, he is a member of the U.S. National Academy of Engineering, a Fellow of the Royal Academy of Engineering in the U.K., the Russian Academy of Sciences and the Royal Swedish Academy of Engineering Sciences.

Robert Ritchie is internationally known for his work in materials science, fracture mechanics and fatigue-crack propagation of a very broad range of materials, from metallic alloys, intermetallics, glasses, ceramics, polymers and composites, to MEMS, implant biomaterials, and biological materials, *e.g.*, bone and teeth. He has published over 700 papers and edited 19 books in the technical literature, with significant impact (*h-index* of 101 on Google Scholar).

His most notable and sustained contribution to the field over the past 40 years or so has been in defining the mechanistic role of microstructure in governing the fatigue behavior of metallic alloys (specifically aluminum, titanium, nickel and especially steels), intermetallics (*e.g.*, α -TiAl), ceramics (PSZ, Al₂O₃, Si₃N₄, SiC) and the interfaces between them, which he presented in terms of his conceptual models involving the mutual competition of intrinsic damage and extrinsic shielding mechanisms.¹ Indeed, he was one of the early pioneers in developing an understanding of the relationships between microstructure and fatigue-crack growth; his work with one of his students, Subra Suresh, in the early 1980s provided one of the first *microstructural* descriptions of crack-tip shielding in terms of models/mechanisms for fatigue crack closure.^{2,3} Using this approach as a framework for the mechanistic understanding of the growth of cracks by fatigue, specifically by defining the separate contributions to fracture resistance by so called intrinsic (*e.g.*, plasticity) and extrinsic (*e.g.*, shielding) mechanisms,⁴ Ritchie also made seminal contributions to such factors as the effect of variable amplitude loading, mixed-mode fatigue, and most notably the role of small cracks.⁵ In the late 1980s to 1990s, he was one of the first researchers to develop an understanding of the cyclic fatigue of brittle materials (ceramics and intermetallics) at both low and elevated temperatures; indeed, his study with his then student Reiner Dauskardt in 1987 was the first to measure the

susceptibility of ceramics to fatigue-crack growth under applied tensile loads.⁶ More recently, he identified, and developed a “reaction-layer” model, for the surprising fatigue failure of mono- and poly-crystalline silicon MEMS.⁷ He is also a leading researcher in the mechanistic understanding of the fatigue and toughness behavior of metallic glasses.^{8,9}

From this work, it is clear that he is one of a few individuals who can bring together the science of materials with the concepts of engineering structures. He works closely with industry and is primarily involved in “real world” problems. As an example, he was chosen by the U.S. Air Force in the late 1990s to head a multidisciplinary university research initiative to examine the failure of gas turbine components by high-cycle fatigue, where he led a team of academic/industrial researchers to address this problem. His contributions have been both broad in a programmatic sense and far reaching in a technical sense, and reflect this balance between science and real-world engineering.

In addition to his work on fatigue, he is also credited with the major contribution to the field of fracture in terms of the so-called RKR model for cleavage fracture.¹⁰ This model, which was arguably the first micromechanics *crack-tip* model for the toughness of metals, was developed in 1973 by Ritchie, his Ph.D supervisor John Knott, and Jim Rice, and is still regarded as the underlying quantitative description of brittle fracture in metallic microstructures, being cited in the literature ~20-40 times each year, some 40 years after its publication. It has been widely applied to describe fracture behavior in metals, laminates and certain brittle solids; indeed, the model has been reconstituted on a statistical basis by a number of different researchers (including Knott and Ritchie¹¹), and most recently Ritchie has adapted it to provide a statistical description of mixed-mode fracture in functionally-graded materials (with the late Rowland Cannon)¹² and of hydrogen embrittlement fracture in steels (with Petros Sofronis).¹³

On a less academic level, Ritchie is also well known for his bioengineering work on the structural integrity of cardiac valve prostheses. Working with virtually all the leading manufacturers of mechanical heart valve implants, in the U.S. and abroad, Ritchie was the first to develop methodologies for predicting the safe lives of such devices, initially for metallic prostheses and subsequently for those manufactured from pyrolytic carbon, which provided a rational basis for quality control.¹⁴ Although initially greeted with some suspicion by several manufacturers, his damage-tolerant lifing approach is now mandated by the FDA for the certification of all prosthetic valves. He is currently interested in life-prediction methodologies for cardiovascular stents, dental implants and MEMS devices.

One of his other current research interests lies with the development of damage tolerance in materials using novel approaches to combine the two generally mutually exclusive properties of strength and toughness.¹⁵ Using the inspiration of Nature, he recently developed, with colleague Tony Tomsia, lightweight ceramic materials infiltrated with a small fraction of a compliant phase (metal or polymer) in the form of a “brick-and-mortar” structure mimicked from the architecture of red Abalone shells (nacre).¹⁶ Using a novel ice-templating processing method, they generated a suite of (bulk) hybrid alumina ceramic structural materials with the highest fracture toughness recorded to date; indeed, the specific strength/toughness properties of their materials were comparable with metallic aluminium. Although the field of biomimetics is currently a very “hot” in the science of materials, this work is one of only a very few examples where a complex biological material could be mimicked, actually made in bulk form, and shown to have unprecedented mechanical properties. Indeed, this approach shows truly excellent promise for the design of new structural materials in the future.

Last but not least, Ritchie has also made major scientific contributions to the mechanistic understanding of the multiscale origins of the fracture resistance of biological materials. He has studied shells and fish scales, but his major contributions have been on teeth¹⁷ and most notably human bone, where he has examined how,¹⁸ and at what structural size-scales,¹⁹ do these materials develop their damage tolerance, and how this can biologically degrade due to aging, therapy and disease.²⁰ Within the hierarchical structure of bone, he has quantified and mechanistically interpreted with a range of techniques (fracture mechanics, synchrotron x-ray tomography, SAXS/WAXD and Raman/FTIR spectroscopy), the origins of intrinsic toughness from plasticity at the nanometers scale and the origins of extrinsic toughness from shielding at the microns scale, and the coupling between them.^{19,20} This work has provided very new and critically important insight into why bones break, not simply from a loss in bone mass, but additionally from a degradation in their hierarchical structure due to biological factors.

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New Computational Methods for Boundary Value Problems

by Timon Rabczuk

Short Biography

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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
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ERC-CoG COMBAT
Coordinator of ITN-INSIST and IRSES-MULTIFRAC*

Abstract 1:

We present a mixed finite element formulation that is coupled with topology optimization to maximize their intrinsic material performance with regards to the energy conversion potential of flexoelectric nanostructures. Using Barium Titanate (BTO) as the model flexoelectric material, we demonstrate the significant enhancement in energy conversion that can be obtained using topology optimization. We also demonstrate that non-smooth surfaces can play a key role in the energy conversion enhancements obtained through topology optimization. Finally, we examine the relative benefits of flexoelectricity, and surface piezoelectricity on the energy conversion efficiency of nanobeams. We find that the energy conversion efficiency of flexoelectric nanobeams is comparable to the energy conversion efficiency obtained from nanobeams whose electromechanical coupling occurs through surface piezoelectricity, but are ten times thinner.

Overall, our results not only demonstrate the utility and efficiency of flexoelectricity as a nanoscale energy conversion mechanism, but also its relative superiority as compared to piezoelectric or surface piezoelectric effects.

Abstract 2:

This paper presents a design methodology based on a combination of isogeometric analysis (IGA), level set and point wise density mapping techniques for topology optimization of piezoelectric/flexoelectric materials. The fourth order partial differential equations (PDEs) of flexoelectricity, which require at least C^1 continuous approximations, are discretized using Non-Uniform Rational B-spline (NURBS). The point wise density mapping

technique with consistent derivatives is directly used in the weak form of the governing equations. The boundary of the design domain is implicitly represented by a level set function. The accuracy of the IGA model is confirmed through numerical examples including a cantilever beam under a point load and a truncated pyramid under compression with different electrical boundary conditions. Finally, we provide numerical examples demonstrating the significant enhancement in electromechanical coupling coefficient that can be obtained using topology optimization.

Abstract 3:

We present an extended finite element formulation for piezoelectric nanobeams and nanoplates that is coupled with topology optimization to study the energy harvesting potential of piezoelectric nanostructures. The finite element model for the nanoplates is based on the Kirchoff plate model, with a linear through the thickness distribution of electric potential. Based on the topology optimization, the largest enhancements in energy harvesting are found for closed circuit boundary conditions, though significant gains are also found for open circuit boundary conditions. Most interestingly, our results demonstrate the competition between surface elasticity, which reduces the energy conversion efficiency, and surface piezoelectricity, which enhances the energy conversion efficiency, in governing the energy harvesting potential of piezoelectric nano structures.

Abstract 4:

We present in this work a coupled XFEM/level set method for the optimization of nanostructures, where our specific interest is in capturing and elucidating surface effects on the optimal nanodesign. XFEM is used to solve the nanomechanical boundary value problem, which involves a discontinuity in the strain field and the presence of surface effects along the interface. The boundary of the nano-structure is implicitly represented by a level set function, which is considered as the design variable in the optimization process, and the shape derivative of the objective function for the nano mechanical problem is derived. Two objective functions, those of minimizing the total potential energy of a nanostructure subjected to a material volume constraint and minimizing the least square error compared to a target displacement, are chosen for the numerical examples. We present results of optimal topologies of a nanobeam subject to cantilever, fixed and simply supported boundary conditions. The numerical examples demonstrate the importance of size and aspect ratio in determining how surface effects impact the optimised topology of nano beams.

Contributions in Carbon Nanotubes Sheets Research

by Ray Baughman

Short Biography

Ray Baughman became the Robert A. Welch Professor of Chemistry and Director of the NanoTech Institute at the University of Texas in Dallas in August 2001, after 31 years in industry. He is a Member of The National Academy of Engineering and The Academy of Medicine, Engineering and Science of Texas; the EU Academy of Sciences, a foreign member of the European Academy of Sciences; a Fellow of the Royal Society of Chemistry, the National Academy of Inventors, and the American Physical Society; an Academician of The Russian Academy of Natural Sciences; an honorary professor of 7 universities in China; and is on editorial or advisory boards of Science and other journals. Ray has 80 issued US patents and 415 refereed publications, with over 32,580 citations and an H-index of 82. He has received the Chemical Pioneer Award of the American Institute of Chemists (1995), the Cooperative Research Award in Polymer Science and Engineering (1996), the New Materials Innovation Prize of the Avantex International Forum for Innovative Textiles (2005), Nano 50 Awards from Nanotech Briefs Magazine for Carbon Nanotube Sheets and Yarns (2006) and for Fuel Powered Artificial Muscles (2007), the NanoVic Prize from Australia (2006), the Scientific American Magazine 50 recognition for outstanding technological leadership (2006), the CSIRO Metal for Research Achievement (2006), the Chancellor's Entrepreneurship and Invention Award (2007), the 21 for the 21st Century award (2007), the Alumni Distinguished Achievement Award of Carnegie Mellon University (2007), the Kapitza Metal of the Russian Academy of Natural Sciences (2007), the Graffin Lectureship of the American Carbon Society (2010), the Tech Titans Award in Education (2011), Time Magazine recognition in 50 Best Inventions of the Year (2011), the SGL Carbon Award of the American Carbon Society (2013), the Tech Titans Technology Inventors Award (2015), the 2015 Inventor Award for Energy Harvesting Materials and Systems, and the R&D 100 Gold Award for Market Disruptor Product (2015). He was named the Honorable Yang Shixiang Professor of Nankai University and the Honorable Tang Aoqing Professor of Jilin University in 2010 and was listed 30th in the Top 100 Material Scientists of the Decade (2000-2010). The Baughman laboratory was established in his honor in China in 2014 at the Jiangnan Graphene Research Institute in Changzhou.

Abstract 1:

By introducing twist during spinning of multiwalled carbon nanotubes from nanotube forests to make multi-ply, torque-stabilized yarns, we achieve yarn strengths greater than 460 megapascals. These yarns deform hysteretically over large strain ranges, reversibly providing up to 48% energy damping, and are nearly as tough as fibers used for bulletproof vests. Unlike ordinary fibers and yarns, these nanotube yarns are not degraded in strength by overhand knotting. They also retain their strength and flexibility after heating in air at 450-C for an hour or when immersed in liquid nitrogen. High creep resistance

and high electrical conductivity are observed and are retained after polymer infiltration, which substantially increases yarn strength.

Abstract 2:

Individual carbon nanotubes are like minute bits of string, and many trillions of these invisible strings must be assembled to make useful macroscopic articles. We demonstrated such assembly at rates above 7 meters per minute by cooperatively rotating carbon nanotubes in vertically oriented nanotube arrays (forests) and made 5-centimeter-wide, meter-long transparent sheets. These self-supporting nanotube sheets are initially formed as a highly anisotropic electronically conducting aerogel that can be densified into strong sheets that are as thin as 50 nanometers. The measured gravimetric strength of orthogonally oriented sheet arrays exceeds that of sheets of high-strength steel. These nanotube sheets have been used in laboratory demonstrations for the microwave bonding of plastics and for making transparent, highly elastomeric electrodes; planar sources of polarized broad-band radiation; conducting applique's; and flexible organic light-emitting diodes.

Abstract 3:

Multifunctional applications of textiles have been limited by the inability to spin important materials into yarns. Generically applicable methods are demonstrated for producing weavable yarns comprising up to 95 weight percent of otherwise unspinnable particulate or nanofiber powders that remain highly functional. Scrolled 50-nanometer-thick carbon nanotube sheets confine these powders in the galleries of irregular scroll sacks whose observed complex structures are related to twist-dependent extension of Archimedean spirals, Fermat spirals, or spiral pairs into scrolls. The strength and electronic connectivity of a small weight fraction of scrolled carbon nanotube sheet enables yarn weaving, sewing, knotting, braiding, and charge collection. This technology is used to make yarns of superconductors, lithium-ion battery materials, graphene ribbons, catalytic nanofibers for fuel cells, and titanium dioxide for photocatalysis.

Abstract 4:

Artificial muscles are of practical interest, but few types have been commercially exploited. Typical problems include slow response, low strain and force generation, short cycle life, use of electrolytes, and low energy efficiency. We have designed guest-filled, twist-spun carbon nanotube yarns as electrolyte-free muscles that provide fast, high-force, large-stroke torsional

and tensile actuation. More than a million torsional and tensile actuation cycles are demonstrated, wherein a muscle spins a rotor at an average 11,500 revolutions/minute or delivers 3% tensile contraction at 1200 cycles/minute. Electrical, chemical, or photonic excitation of hybrid yarns changes guest dimensions and generates torsional rotation and contraction of the yarn host. Demonstrations include torsional motors, contractile muscles, and sensors that capture the energy of the sensing process to mechanically actuate.

Abstract 5:

The high cost of powerful, large-stroke, high-stress artificial muscles has combined with performance limitations such as low cycle life, hysteresis, and low efficiency to restrict applications. We demonstrated that inexpensive high-strength polymer fibers used for fishing line and sewing thread can be easily transformed by twist insertion to provide fast, scalable, nonhysteretic, long-life tensile and torsional muscles. Extreme twisting produces coiled muscles that can contract by 49%, lift loads over 100 times heavier than can human muscle of the same length and weight, and generate 5.3 kilowatts of mechanical work per kilogram of muscle weight, similar to that produced by a jet engine. Woven textiles that change porosity in response to temperature and actuating window shutters that could help conserve energy were also demonstrated. Large-stroke tensile actuation was theoretically and experimentally shown to result from torsional actuation.

Abstract 6:

Superelastic conducting fibers with improved properties and functionalities are needed for diverse applications. Here we report the fabrication of highly stretchable (up to 1320%) sheath-core conducting fibers created by wrapping carbon nanotube sheets oriented in the fiber direction on stretched rubber fiber cores. The resulting structure exhibited distinct short- and long-period sheath buckling that occurred reversibly out of phase in the axial and belt directions, enabling a resistance change of less than 5% for a 1000% stretch. By including other rubber and carbon nanotube sheath layers, we demonstrated strain sensors generating an 860% capacitance change and electrically powered torsional muscles operating reversibly by a coupled tension-to-torsion actuation mechanism. Using theory, we quantitatively explain the complementary effects of an increase in muscle length and a large positive Poisson's ratio on torsional actuation and electronic properties.

Achievements in Biological Physics & Applied Biophysics

by Erich Sackmann

Short Biography

Biographical Sketch:

Erich Sackmann received his Diploma in Physics in 1961 and did his PHD in Physics 1964 with Professor Theodor Förster from the Technical University of Stuttgart. After two years as Member of Technical Staff at Bell Telephone Laboratories in Murray Hill he worked as research assistant at the Max Planck Institute for Biophysical Chemistry in Göttingen. He did his Habilitation in Physical Chemistry at the University of Göttingen.

1974 he became Full Professor of Physics and head of the biophysics department at the University of Ulm. From 1980 to 2003 he held the chair of Biological Physics at the Physics Department of the Technical University Munich. He presently works as Professor Emeritus at the Technical University Munich and the Ludwig Maximilian University Munich.

Professional Activities:

Prof Sackmann served in numerous national and international committees including RIKEN Institute in Japan, Institute Curie Paris, Max Planck Society and Institutes, Minerva Centers, Heräus Foundation, Helmholtz Excellence Programs. He served as founding Editor of "European Biophysic Letters" as editor of Biological Physics Section of "Progress in Physics" and as Advisory Board member of ChemPhysChem. He is presently on the Editorial Board of Acta Materialia Biophysica and Physical Review. E

From 1974-1980 he was President of the German Biophysical Society. He was a founding member and chairman of the Biological Physics Section in the German Physical Society (DPG) and from 1989-1991 served as Dean of the Faculty of Physics of the Technical University Munich. From 1988-2000 he served as Chairman of the DFG "Sonderforschungsbereich 266 (Interdisciplinary Research Project): Biological and Artificial Interfaces on Solids".

Awards

2001 Oswald Award, German Colloid Society

Fellow of the American Physical Society 2002

2004 Regents professorship of University of California (UCLA)

2006 Stern-Gerlach Medal of the Deutsche Physikalische Gesellschaft

Research Fields

1962-1965 NMR spectroscopy of ^{13}C -H-spin-spin coupling mechanisms in organic molecules.

1967-1975 (a) Liquid Crystals: Scientific and practical applications (b) Photophysics of organic single crystal.

1972-1995 Biological Physics: Bottom-up design of mimetics of biological composite membranes to study (i) the physical basis of the self-assembly of functional domains in membranes and (ii) of the physics of cell adhesion.

1995-2000 Physical basis of the biological function of (passive and active) actin-based intracellular macromolecular scaffolds based on the comparative studies of the viscoelastic impedances of *in vitro* models and living cells.

1995-2017 Physics of the Cell. (i) Physical basis of cell adhesion and polarized cell migration in tissue (ii) Logistically controlled self-assembly of intracellular functional machines-(iii) Analogies between technical and biological control systems.

>2003- Bionics: Biological evolution as interplay of physics and genetics- Learning from nature to overcome evolutionary crises.

A. Main achievement From PHD to Habilitation: a summary

During my PHD and Habilitation I worked on three fields:

First, NMR studies of indirect ^{13}C -H Spin Spin coupling of organic molecules. Second, scientific and practical application of Liquid Crystals. Third, photophysics of aromatic organic crystals composed of charge transfer complexes and excimer forming aromatic molecules.

In the Part I developed the first method to measure both the absolute values and the sign of indirect CH-coupling constants, yielding new insights into intramolecular coupling by Hunds rule and Fermi contact interaction [1].

In Part II, I discovered magnetically induced cholesteric-to-nematic transition and developed methods to determine order parameter tensors and orientation of electronic transition moments of aromatic chromophores in ordered nematic phases.

In Part III we developed methods to measure the mobility of triplet excitons of charge transfer crystals for the first time.

B. Switching to Biological Physics.> 1972

In 1972 I switched from liquid crystal (LC) physics to biological physics motivated by the intuition that evolution, self-assembly and function of living matter is guided by physics, and that the best strategy to study this fundamental question would be the bottom-up approach by designing biomimetic systems fulfilling bio-analogue functions. Coming from LC-physics we started with biological membranes since we recognized to be multicomponent 2D smectic liquid crystals composed of bilayers of amphiphatic lipid molecules and integrated proteins.

Our research focused on the question how order can be formed in multi-component lipid-protein alloys of natural membranes. New methods were developed to determine phase diagrams of lipid-protein alloys. We introduced Small Angle Neutron Scattering (SANS) combined with contrasts matching techniques into the field and showed that SANS is the only technique enabling the determination of phase diagrams in thermal equilibrium. These efforts led us to propose a "heterogeneous shell model" postulating that order in multicomponent lipid-protein alloys is generated by phase separation mediated selective lipid protein interaction mechanism. Our model contrasted, with the "fluid mosaic model" favored by biologist which was based on the assumption that lipids play only a passive role as solvent. After the discovery of "rafts" (around 1995) the heterogeneous shell model is now generally accepted.

[1] (a) E. Sackmann and Träuble J. Amer. Chem. Soc. 94, 4499 (1972). (b) A. Stier and E Sackmann. Biochim et Biophys. Acta, 311 (1973) (c) Sackmann, Galla et al Biochemistry (1973) and, 5360.

[2] State of the art summary 1995; (a) E. Sackmann Chapter I and V in Handbook of Biological Physics (Sackmann and Lipowsky eds) Elsevier 1995 (b) E. Sackmann J. Phys.: Condens. Matter 18 (2006) R785–R825.

C. Dynamics of Membranes- from 10^{-11} -1 sec

The second field of membrane research pioneered by us is the evaluation membrane dynamics starting with the first demonstration that bio-membranes are two dimensional fluids. After the early measurements of lipid diffusivities by spin labels [Träuble and Sackmann 1972] and excimer forming probes [Galla et al 1973] we pioneered the introduction of quasi-elastic neutron scattering (QENS) combined with contrast matching as unique tool to study membrane dynamics from μsec to seconds. By making use of the unique possibility to measure incoherent scattering factors we could measure the short range and long range lateral diffusion of lipids and the motion of side chains and hydrocarbon chain defects (kinks) along the hydrocarbon chain. We showed that lipid diffusion in membranes is determined by the free volume model, [3b and 3c, König, 1992]) allowing us to study correlations between membrane density and molecular motions, We finally demonstrated the breakdown of Saffman-Delbrück logarithmic law of diffusion in membranes close to solid surfaces by frictional coupling of membranes

with rigid substrates. We showed that the diffusion coefficient depends is inversely proportional to the square of the radius enabling high precision measurements of protein radii (Evans and Sackmann, 1988).

D. Bending Elasticity Concept of Cell Shape

We provided the first direct experimental proof of the bending elasticity concept of cell shape by demonstrating that the well-known transitions between disc shaped and cup-shaped red blood cells or membrane budding processes can be mimicked by single component lipid bilayers by simply increasing the area-to-volume ratio, whereas asymmetric shapes are formed by interplay of bending and shear elasticity which introduces a new length scale determined by the ratio of the elastic moduli, Summary; E. Sackmann (1994) 7th DATTA Lecture FEBS Letters 346, 3-16.

In this context we developed several new techniques for high precision measurements of bending moduli of vesicles and cells, all of them depending on the parallel development of fast image processing, at times when such devices were not yet available commercially. Two major techniques involve : (i) measurements of bending moduli as function of wavelength by Fourier analysis of contour fluctuations.(ii) High Frequency electric field deformation based on the Maxwell-Wagner polarisation concept . (a) Engelhart et al (1985) J. Physique Letters. **46**, L-395- L-400. (b) J. Engelhardt and E. Sackmann (1988). Biophys. J 54, 495-508(b)J. Rädler et al (1995) Phys. Rev. E 51 4526-4536.M Peterson et al).

E. Applied Biophysics: Supported membranes; Scientific and Practical Applications (1995)

Starting in 1992 we pioneered the bottom-up design of bio-functional interfaces on solid state devices based on supported membranes separated from the solid by soft and hydrated ultrathin polymer cushions.

One central aim was to fabricate bio-analogue environments for the non-denaturing immobilization of proteins and cells with the major aim of designing mimetics of cell or tissue surfaces for studies of the physics of cell adhesion and cell locomotion under biomimetic conditions.

The second aim was to design biosensors on electro-optical devices for signal detection with high sensitivity surface sensitive techniques Surface Plasmon Resonance on Si and GaAs in the near Infrared and dynamic conductivity.

The major advantages of the design concept is that the organization of the components can be manipulated by 2D electrophoresis and that it allows to study fundamental properties of lipid/protein bilayers by powerful surface sensitive techniques. of the sensor device. (a) E. Sackmann (1996) Science 271, 43-48 (b) M. Tanaka and E. Sackmann Nature 437,656 (2005).

F. On the Physics of Cell Adhesion: Comparative studies of biomimetic systems and cells

We developed a versatile model systems for quantitative studies of cell adhesion based on the, quantitative reflection interference contrast microscopy (RICM) combined with fast 2D image processing system. It allowed us to reconstruct the cell shape close to the surface and to measure first, interfacial distances and local contact with nm spatial and msec temporal resolution and secondly free adhesion energies of adhesion as function of membrane elastic moduli

Together with Robijn Bruinsma, Alexej Boulbitch, Udo Seifert and Ana Smith we showed for the first time that cell adhesion is controlled by the antagonistic interplay between (i) strong short range attraction forces and (ii) medium range repulsive forces induce by large polyelectrolyte brushes forming the cells glycocalix and (iii) long range repulsive forces generate by the bending undulation induced cell surface roughness. We further showed that

cell adhesion is inevitably followed by the decay of the adhesion zone in small domains of tight adhesion formed by clustering of the CAMs (Integrin) separated by weakly adhering zones. We finally established analogies between cell adhesion and the Cahn theory of first order heterogeneous wetting. A further novel result is that The free energy of adhesion is determined by the osmotic equilibrium of bound receptors with the reservoir of free receptors (in the membrane) which may result in the reduction of the adhesion strengths by several orders of magnitude. (Nardi et al, 1999).

Recent reviews; (i) E. Sackmann and A. Smith Physics of cell adhesion: some lessons from cell mimetic systems Soft Matter, 2014, 10, 1644. (ii) ES Lecture Physics of Cell Adhesion. Lecture can be downloaded via www.biophy.de

G. Viscoelastic Impedance and Biological Function of in-vitro and in vivo actin networks

The intracellular actin scaffold consisting of filamentous actin and associated regulatory proteins is not only an essential cellular organelle but also a versatile model system to study the physics of macromolecular networks for two reasons. First, single filaments can be directly observed, enabling us to directly relate dynamic elastic properties to molecular motional processes. Second, a manifold of natural network regulating proteins is available to manipulate the structure and function of the networks.

We entered the field of cell physics by studying in vitro models of the actin cortex starting 1998. The highlights of these efforts are;

- First parallel measurement of the nucleation and growth of entangled actin networks by QELS (Schmidt et al, 1989) and a newly developed high sensitivity torsional micro-rheometer (Müller et al, 1991). These experiments triggered the rapid development of new theories of the physics of semiflexible macromolecular networks by various theoretician, notably Toni Maggs, Erwin Frey, Klaus Kroy, David Morse, Fred MacKintosh and J. Prost),
- The direct experimental verification of the tube model of polymer networks and the concept of reptation by microfluorescence techniques (Käs et al, 1994) and by a novel nm-resolution colloidal probe microscopic technique (Dichtl et al 2000). We further determined the interaction potential between the filaments and the tube wall as well as tube diameter fluctuations (Dichtl et al 2000).
- In 2000 we designed mechanical models of composite cell plasma by developing a method to self-assemble entangled and cross-linked actin corteces beneath the surface of giant vesicles (Häckl et al, 1999, Limozin 2002). By application of our high resolution colloidal force microscopy we could measure the viscoelastic impedance of the biomimetic actin cortex between 0.05 sec and 10sec showed that the viscoelastic impedance of these model cell closely resembled that of entangled actin networks state (Roth et al 2005)
(a) R. Götter et al *Macromolecules*, 29, 30–36; (b) Hinner, et al (1998) *Phys. Rev. Lett.* 81, 2614. (c) Limozin et al. (2002) *Phys. Rev. Lett.* 16 168103-1- (d) A, Roth L. Limozin (2005) *Phys. Rev Lett.* 95, 178101 (2005) (e) Tempel et al. (1996) *Phys Rev E* 54, 1802.

H. Cells as Tensegrity Structures-Shell-Spring-Model of cells

By application of magnetic tweezer microrheometry we showed first, that the cytoplasm is an active viscoplastic body and second, that its function and mechanics is determined by crosstalk between the membrane associated actin network and the aster shaped microtubule system. This mechanical design shares several features with the Buckminster Fuller tensegrity structures, such as the mechanical stabilization by pre-stressing the MT-ropes and the elastic shell [Heinrich 2006]. The mechanical design is extreme robust and cells can return to the

resting state even after very strong deformations such as during the locomotion through narrow blood capillaries.

The cytoplasm space is a very soft viscoplastic fluid: an absolute necessity to ensure rapid intracellular material transport by vesicles. Together with my colleagues we developed a method allowing us to separate directed motion on microtubules and random walks (Arcinet et al) which allowed us to measure intracellular viscosities and forces mediated by MT-based motors.

(a) D. Heinrich and E. Sackmann (2006) *Acta Biomaterialia* 2, 619–631). (b) Arcinet et al (2014) *Phys Rev. Lett.* 101, 248103

I. Physics of Globally Directed Cell Migration

In 1995 we developed the RICM technique into a versatile tool to study cell migration on weakly adhering bio-functional surfaces. We showed that cells migrate by stepwise advancement of the front, driven by solitary actin gelation pulses followed by retraction of the end (uropod). We further showed that cyclic progression is coordinated in time and space by the antagonistic interplay of two molecular switches: the GTPases RhoA and Rac1. Interestingly, broad protrusions and fingerlike filopodia may form in parallel (such as at the front of axon growth cones) which is a consequence of the lateral inhibition of the GTPases.

Based on our long standing experiments on cell migration and a survey of literature we showed that the directed motion is controlled by global cell polarization through the interplay of microtubules with the actin cortex mediated by passive and active supramolecular actin/MT-complexes and associated global Ca^{++} -gradients [Sackmann 2015] .

In a separate set of experiments we showed that the cell locomotion along slender objects is driven by travelling solitary actin gelation waves (SAGW), which are guided by travelling clouds of the high affinity lipid anchors PI-3,4,5-P3 which are generated by local activation of the generator PI-3K and annihilated by the PI-3,4,5-P3 annihilator PTEN .

E. Sackmann, F. Keber and D. Heinrich (2010). *Annu. Rev. Condens. Matter Phys* 1: 257

E Sackmann *Biochim Biophys Acta* 1853 (2015) 3132–3142. E. Sackmann, F. Keber and D. Heinrich (2010). *Annu. Rev. Condens. Matter Phys*1: 257

Recent Scientific activities

J. Logistic self-assembly of functional assemblies and biological control system

Our studies of the physical basis of cell adhesion and locomotion led to a new concept of logistic self-assembly of functional entities at cell membranes. We showed that functional machines at membrane surfaces self-organize by logistically controlled recruitment of functional modules at specific sites. From the point of view of physics most interesting is that the self- organization is mediated by electrostatic and hydrophobic interfacial forces, which are switched-on by external forces or signals, such as Ca^{++} -bursts or the generation of highly charged affinity lipid anchors acting as second messengers.

These studies teaches us that biological control systems share many features with technical ones but are far superior concerning three aspects: first, they can optimize the material properties of tissue to maximize the life time of cells or functional machines. Secondly, they can adapt the material properties of cells and tissue, such as viscoelastic moduli, in an interactive way to balance forces between cells and tissue. Thirdly, they can repair damages.

We are convinced that studies of natural control systems can teach us how to transfer the strategies of logistic control of self-organization and self-repairing to technical system by bottom-up approach.

Physicists can contribute to this field in two ways. First, by developing novel nanoscopic measuring techniques and secondly by foster more systemic thinking in the field by searching for universal regulatory systems.

Physicists are often frustrated by the complexity of proteins forming supramolecular

functional complexes. However to contribute to the advancement to of physics of living matter cells it is absolutely necessary to become familiar with natures strategy to of control systems. Most importantly their task is to bring in more systemic and quantitative thinking into life sciences

J. Biological Evolution as interplay of Physics and Genetics-or Nature as Material designer

Mother Nature achieved the evolution of a sheer infinite manifold of living beings with an astonishingly small number of organic molecules by interplay of physics, and genetics, combined with the concept of hierarchical design principles. Nature was most inventive during evolutionary crises mediating quantum jumps of evolution.

Many concepts of human rational design of smart materials were invented by nature many million years ago. A major motivation for our work on evolution and physics is to show that Nature can teach us how to design highly sophisticated mechanical structures and systems comprising length scales from 10-10¹⁰ nm by hierarchical design from functional modules (such as lipid membranes, ion pumps and molecular *motors* E, Sackmann(2013). *Int. J. Nanotechnology* **10** 376-389 *ES Lecture Notes on Biological Physics/Bionics, Biomineralization* (www.biophy.de).

K. Teaching: Motivation and Aims

The switching to biological physics was guided by the desire to open new fields for young physicists in research and industry. After my appointment as the first holder of a Biophysics Chair in a Physics Department in Germany (at the University of Ulm) I developed a curriculum on Biological Physics for physicists and biochemists a four semester course including laboratory courses. Teaching was based on a manuscript now available as Textbook in German (Sackmann and Merkel Lehrbuch der Biophysik Wiley Verlag 2009). Numerous special lectures are collected in ES. Lecture Notes in Biological Physics-available via www.biophy.de

A reliable measure of the success of a new fields in physics is whether students get good job offers in industry. Here we were especially successful. Many of these students got excellent job offers (i) owing to their knowledges in classical physics (ii) their highly developed capacity for interdisciplinary cooperation and (iii) their motivation to cooperate with engineers and life scientists, About five of the students successfully started new companies.

Concerning the Necessity to Become Familiar with Cell Signaling in Biological Physics.

The clarification of the control of the structure and function of cells by endogenic und exogenic forces and signalling molecules is absolutely necessary to explore the origin of sicknesses caused by dysfunctions or mutations of biomolecules. Physicists can contribute to life sciences in two ways: first, by developing novel nanoscopic measuring technique and secondly by fostering more systematic thinking in the field, such as by searching for universal features of regulatory systems.

Physicists are often frustrate by the complexity of proteins forming supramolecular functional complexes. However to contribute to the understanding of the design and function of living matter it is absolutely necessary to become familiar with natures strategy of logistic design of complex material of stunning complexity. Moreover, the physicists task is to bring in more systematic and quantitative thinking into the life sciences.

Organometallic Transition Metal Chemistry & Carbon Chemistry

by Malcolm Green

Short Biography

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

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 University

Emeritus Fellow of Balliol College and St Catherine's College

Publications

Two text books, 646 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) Karl Ziegler Prize (German Chemical Society). 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 Society of 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

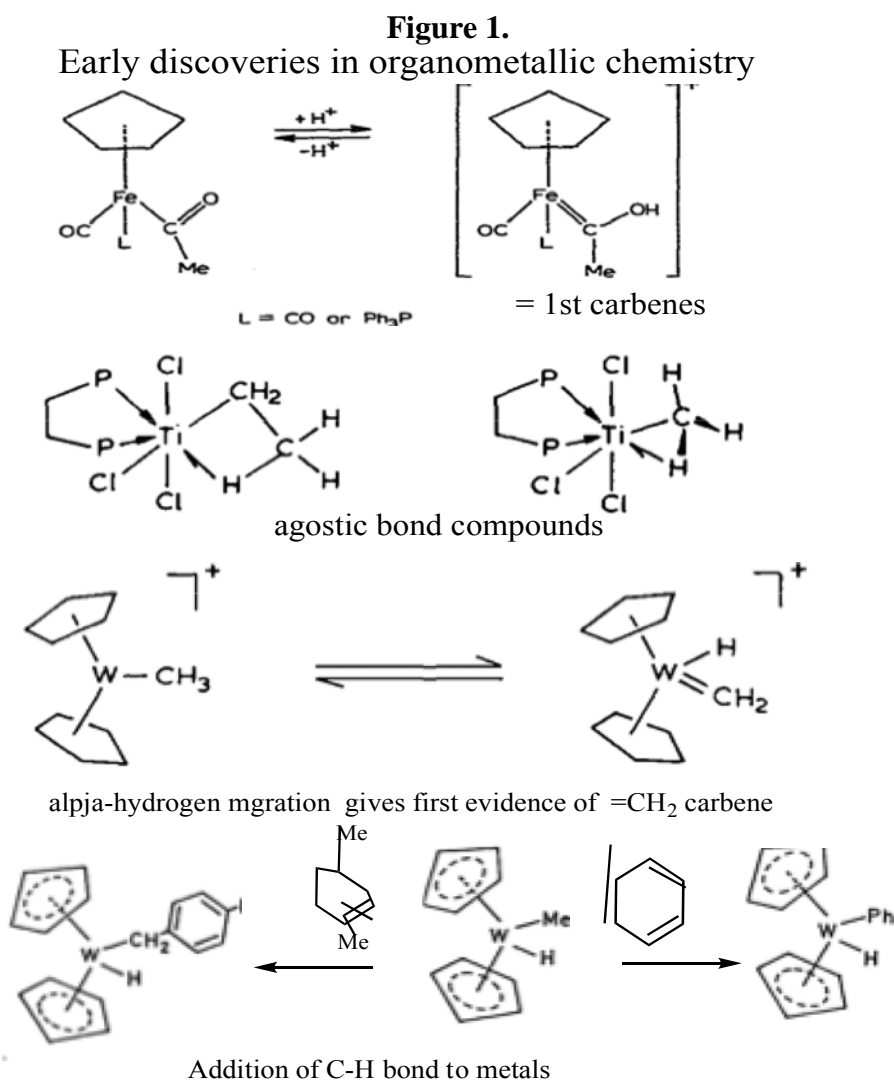
2000 Sir Geoffrey Wilkinson Medal and Prize, (Royal Society of Chemistry)

2001 Lewis Lecture, Cambridge UK FMC Lecturer, Princeton

2002- 2014	<i>Distinguished Visiting Professor, Hong Kong University.</i>
2002	<i>Distinguished Lecturer in Inorganic Chemistry, University of North Carolina</i> <i>34th Canille and Henry Dreyfus Lecturer, Dartmouth College</i>
2004	<i>Honorary Professor of the University of Wuhan (PRC)</i> <i>Bert and KeggieVallee Visiting Professor, Harvard University, March 2004</i>
2006	<i>Falk Plaut Lectureship, 2006. Columbia University NY</i> <i>Honorary Doctorate Southampton University.</i>
2007	<i>Prix Franco-Britannique, Societ�, Francaise de Chemie.</i>
2014	<i>Doctor of Science honoris causa 14/7/2014, University of Warwick.</i>
2015 :	<i>European Prize for Organometallic Chemistry 2015</i>

1. Organometallic Transition Metal Chemistry

This was the first area of research and resulted in the synthesis and new reactions, for example the synthesis of the first zerovalent compounds of the elements Ti, Zr, Hf, Nb and Ta. The synthesis of the second example of a dinitrogen transition metal compound was achieved, as was the discovery of the first unambiguous examples of agostic M-H-C bonds of transition metal compounds and proposal of their role in catalysis. Examples of these reactions are shown in the Figure 1.; the diagrams are copied from the original publication.



2. Homo- and Heterogeneous Transition Metal Catalysts

A mechanism for ethylene polymerization has been described and accepted.

A ruthenium based catalyst for the partial oxidation of methane which was the first stable and highly active and selective catalyst for reaction of methane and oxygen to give hydrogen and carbon monoxide in over 90% yield. This work stimulated a major study in this area.

Also, the discovery of an exceptionally stable and active catalyst for the Fischer-Tropsch reaction which is in now the basis of a new technology for a small-scale F-T biomass –to-hydrocabons industry. The company Velocys was founded based on the patent for the new catalyst and has recently built a plant in Oklahoma City.

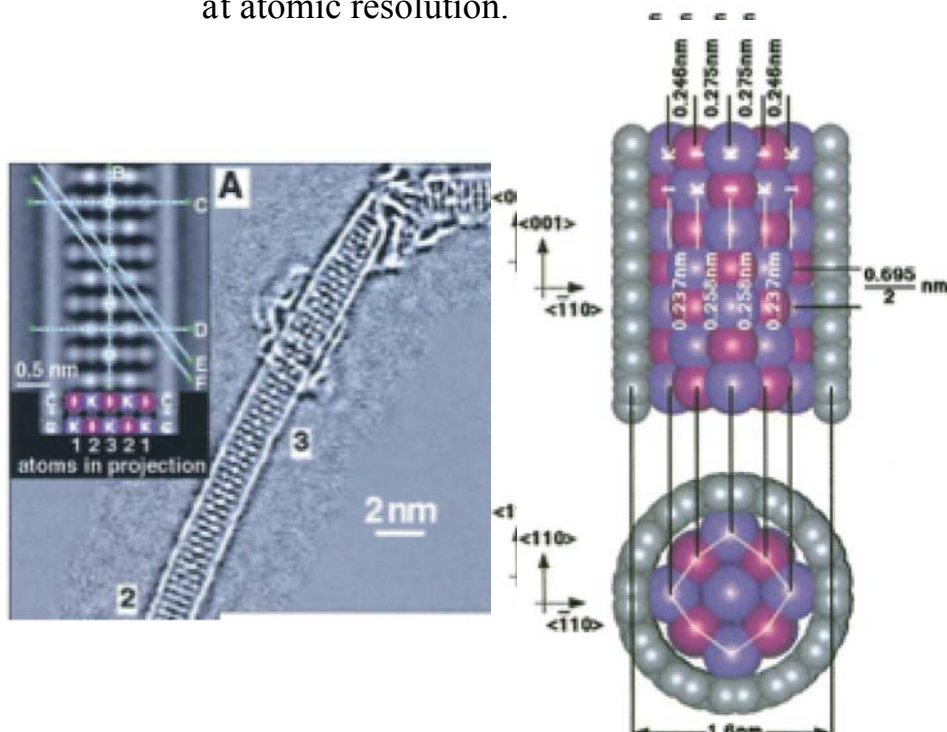
3. Carbon Chemistry.

The first organometallic compounds of C_{60} have been prepared.

Extensive studies have been made of synthesis, purification, opening and filling, reversible corking and chemical functionalization of carbon nanotubes.

Figure 2 below shows a single wall tubes filled with potassium iodide.. Single wall carbon nanotubes filled with radioactive iodine and covered outside with attached organic sugar molecules have been shown to be non-toxic when injected into mice and to be selectively located in their lungs. This work opened the door to a potential method for selective location of nanotubes filled with drugs or imaging agent. Also, single wall carbon nanotubes distributed in silica has given a glass which has exceptional strength.

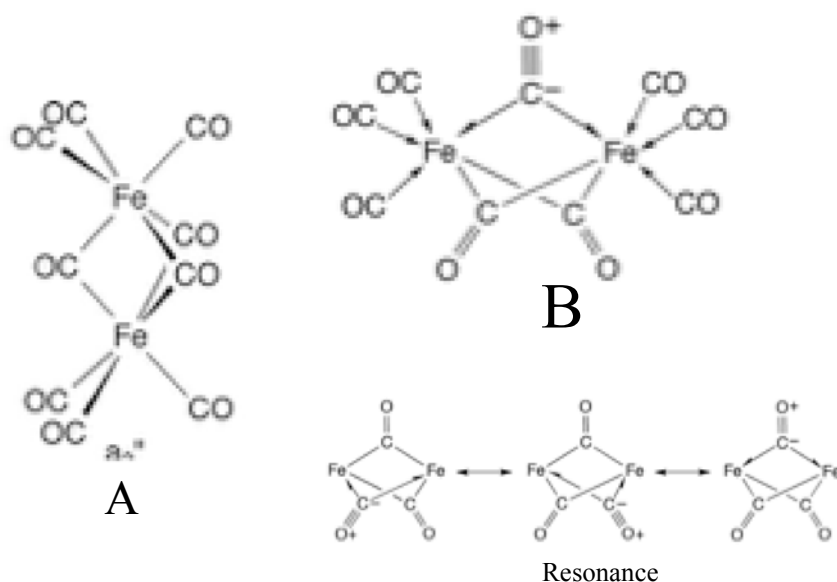
Figure 2. Potassium iodide in a single wall carbon nanotube at atomic resolution.



4. In the recent years I have been developing a new method for the classification and representation of covalent compounds of all elements. This provides a new approach for the teaching chemistry and within the last 5 years many of the top universities in the US and UK have started to teach the Covalent Bond Classification (CBC) to both undergraduates and graduates. Further it is now appearing in major text books. During the development of this new approach it became apparent that there were several new chemical bonds which have not been previously discovered. For example, there are actually 6 different three center - two electron bonds. This is three more than previously known.

An example is the μ -L bond. This occurs on the well known di-iron-eneacarbonyl compound $\text{Fe}_2(\text{CO})_9$ which for over 25 years has been drawn with the structure A in Figure 3 with a single bond between the iron atoms. The electron count for this structure would be 18 electrons for both iron atoms and the molecule should be, as observed, diamagnetic. However over the last 20 years or more theoreticians have said that there was no Fe-Fe bond. This dilemma is solved by the discovery that one of the bridging carbonyl groups is not acting as a bridging ketone forming two $2e-2c$ bonds but rather that one CO is acting as a μ -L bond which gives two electrons to each iron. The correct structure of the diamagnetic, no-single bond structure and an electron count of 18 is shown in the Figure 3. B.

Figure 3. A The original representation of the bonding in $\text{Fe}_2(\text{CO})_9$ with no Fe – Fe bond.
B the correct representation with no Fe – Fe bond.



Recent Achievements in Computational Chemistry

by Robert Benny Gerber

Short Biography

Professor Emeritus of Chemistry, Hebrew University of Jerusalem; Professor Emeritus of Chemistry, University of California at Irvine.

Education: B.Sc. (Chemistry), Hebrew University of Jerusalem (1965); D.Phil., University of Oxford (1968), Advisor: Prof. C.A. Coulson; Postdoctoral Research Associate, Harvard University (1968-69), Advisor: Prof. M. Karplus.

Academic positions:

Senior Researcher, Weizmann Institute of Science (1969-75); Associate Professor (1976); Professor (1980); Saerree K. and Louis P. Fiedler Professor Chemistry (from 1989); Emeritus from 2012), Hebrew University of Jerusalem; Professor of Chemistry (from 1990), University of California at Irvine (Emeritus from 2014); Finland Distinguished Professor, University of Helsinki (2011-2015).

T.K. Roy, R. Sharma and R.B. Gerber

First-Principles Anharmonic Quantum Calculations for Peptide Spectroscopy: VSCF Calculations and Comparisons with Experiment
Phys. Chem. Chem. Phys. 18, 1607-1614 (2016).

Abstract:

First-principles quantum calculations for anharmonic vibrational spectroscopy of three protected dipeptides are carried out and compared with experimental data. Using hybrid HF/MP2 potentials, the Vibrational Self-Consistent Field with Second-Order Perturbation Correction (VSCF-PT2) algorithm is used to compute the spectra without any ad hoc scaling or fitting. All of the vibrational modes (135 for the largest system) are treated quantum mechanically and anharmonically using full pair-wise coupling potentials to represent the interaction between different modes. In the hybrid potential scheme the MP2 method is used for the harmonic part of the potential and a modified HF method is used for the anharmonic part. The overall agreement between computed spectra and experiment is very good and reveals different signatures for different conformers. This study shows that first-principles spectroscopic calculations of good accuracy are possible for dipeptides hence it opens possibilities for determination of dipeptide conformer structures by comparison of spectroscopic calculations with experiment.

L. Partanen, G. Mudachaew, R.B. Gerber and L. Halonen

Temperature and Collision Energy Effects on Dissociation of Hydrochloric

Acid on Water Surfaces

Phys. Chem. Chem. Phys. 18, 13432-13442 (2016).

J. Kalinowski, E.S. Foreman, K.M. Kapnas, C. Murray and R.B. Gerber

Dynamics and Spectroscopy of CH₂OO Excited Electronic States

Phys. Chem. Chem. Phys. 18, 10941-10946 (2016).

A. Cohen and R.B. Gerber

A Noble-Gas Hydride in a Nitrogen Medium: Structure, Spectroscopy and Intermolecular Vibrations of HXeBr@ (N₂)₂₂

J. Phys. Chem. A (Festschrift for R. Kosloff) 120, 3372-3379 (2016).

R. Knaanie, J. Sebek, M. Tsuge, N. Myllys, L. Khriachtchev, M. Räsänen, B. Albee, E.O. Potma and R.B. Gerber

Infrared Spectrum of Toluene: Comparison of Anharmonic Isolated-Molecule Calculations and Experiments in Liquid Phase and in a Ne Matrix

J. Phys. Chem. A (Festschrift for R. Kosloff) 120, 3380-3389 (2016).

B. Hirshberg and R.B. Gerber

Formation of Carbonic Acid in Impact of CO₂ on Ice and Water

J. Phys. Chem. Lett. 7, 2905-2909 (2016).

Abstract:

A new mode of formation is proposed for carbonic acid in the atmosphere. It involves impact of vibrationally excited gas-phase CO₂ molecules on water or ice particles. This is a first mechanism that supports formation on ice as well as on liquid water surfaces. Results of ab initio molecular dynamics simulations are presented on collisions of CO₂ with (H₂O)_n clusters (n = 1, 4, 8, 12). Efficient formation of carbonic acid is seen with product lifetimes exceeding 100 ps. The reaction is feasible even for collision of CO₂ with a single water molecule but in a different mechanism than for larger clusters. For clusters, the transition state shows charge separation into H₃O⁺···HCO₃⁻, which transforms into neutral carbonic acid as the product, hydrated by the remaining waters. Possible atmospheric implications of the results are discussed.

D. Shemesh, S.A. Nizkorodov and R.B. Gerber

Photochemical Reactions of Cyclohexanone: Mechanisms and Dynamics

J. Phys. Chem. A (Festschrift for M.S. Gordon) 120, 7112-7120 (2016).

Abstract:

Photochemistry of carbonyl compounds is of major importance in atmospheric and organic chemistry. The photochemistry of cyclohexanone is studied here using on-the-fly molecular dynamics simulations on a semiempirical multireference configuration interaction potential-energy surface to predict the distribution of photoproducts and time scales for their formation. Rich photochemistry is predicted to occur on a picosecond time scale following the photoexcitation of cyclohexanone to the first singlet excited state. The main findings include: (1) Reaction channels found experimentally are confirmed by the theoretical simulations, and a new reaction channel is predicted. (2) The majority (87%) of the reactive trajectories start with a ring opening via C–C α bond cleavage, supporting observations of previous studies. (3) Mechanistic details, time scales, and yields are predicted for all reaction channels. These benchmark results shed light on the photochemistry of isolated carbonyl compounds in the atmosphere and can be extended in the future to photochemistry of more complex atmospherically relevant carbonyl compounds in both gaseous and condensed-phase environments.

G. Murdachaew, G.M. Nathanson, R.B. Gerber and L. Halonen
Deprotonation of Formic Acid in Collisions with a Liquid Water Surface
Studied by Molecular Dynamics and Metadynamics Simulations
Phys. Chem. Chem. Phys. 18, 29756-29770 (2016).

In Situ Instrumentation for Scaling Fracture

by William Gerberich



Short Biography

*Professor of Chemical Engineering and Materials Science
University of Minnesota, Minneapolis*

Published over 500 peer-reviewed research papers with more than 30 cited over 100 times having an overall h-index of 64. With over 100 PhD and MS students graduated, mostly PhD, of the latter 14 have gone to Academic positions.

Awards

- 2006 – G.E Distinguished Lecture Series, Rensselaer Polytechnic*
- 2006 – Named Honorary Symposium The Materials Society, San Antonio*
- 2002 – Res Mechanica Chair, Leuven, Belgium*
- 1997-2003 – Advisory and Scientific Boards of 6 International Journals*
- 1995- Best Paper Award, International thermal spray conference, High Temp. Soc. of Japan*
- 1994- Outstanding Paper Award, Acta Materialia*
- 1986-1989 –Board Chairman, Acta Metallurgica Publications*
- 1983-1986 – Acta Metallurgica Board of Directors*
- 1980-1988- Mat's Rev. Board, Argonne National Laboratories*
- 1978-1983-Vice Chair, ASTM E9.01 Reseach Committee on Fatigue*
- 1978-1979- Chair ASM Committee on Fracture Mechanics –Metals Handbook*
- 1968 - William Sparagen Award of the American Welding Society*

Extras

- Visiting Professor, ETHZ Zurich, (2013)*
- National Academy of Science Review of NIST (2010)*
- Thomson-Reuters Highly-Cited Materials Science Publication List (2009)*
- Fellow of The Materials Research Society (2012-)*
- Fellow of The Materials Society (2009-)*
- Co-Editor of Fract. Nanomechanics, Vol.119/120, Int.J. Fract. 299-499 (2003).*
- Fellow of the American Society of Metals (1986-)*
- Board of Governors, NSF Institute for Mechanics and Materials, Chair (1994)*
- Board of Governors, NSF Institute for Mechanics and Materials, U.C. San Diego (1992-1994)*
- Consultant to Los Alamos National Labs, Cardiac Pacemakers, Medtronic Inc.(1990-2010)*
- Advisor to the Minnesota Pollution Control Agency, Lakehead Pipeline Co. and Governors Commission on Pipeline Safety.(1986-1987)*
- Advisor to the Director of Public Safety, State of Minnesota (1971-1973)*

Four Careers

For an experimentalist fascinated with fracture, it was a simple matter to change focus (one had to, to keep up with the often changing goals in any given government agency).

The latest instrument on the market or application of established ones given new discoveries provided that. This led to four areas described as the *very large, the very quiet, the very small, and classical mechanics weds atomistics*. In the following, references from our students are almost exclusively utilized

I-The Very Large (1960-1970s):

In the early 60's possessed with the urge to participate in the space race, as a pre-Doc with a Masters degree, an opportunity to join the Jet Propulsion Laboratory(JPL) in Pasadena, CA. led to working on solid propellant engines. One part of this was to analyse the dynamic, non-linear deformation at crack tips using an *in-situ* photoelastic coating technique. This allowed the plastic strain energy to be determined from:

$$U_p = t \int_0^{r_p} \sigma_p \int_0^{2\pi} W_d(r, \theta) r dr d\theta \tag{1}$$

where t is thickness, r_p is the plastic zone and W_d is the strain energy density. This led to an interest by both Professor Max William and his student Jerry Swedlow of Cal Tech, where I was fortunate as a pre-Doc to present my first Academic Seminar.

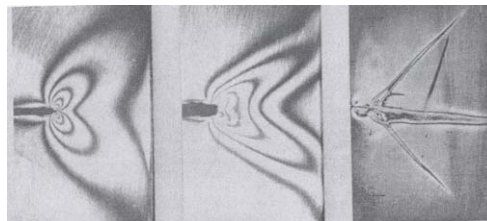


Figure 1: Isochromatics for 2024-T3 Al, 6061-T6 Al and mild steel measuring residual plastic strains (Ref. 1)

The impetus for doing basic research at JPL was to improve the survival rate of rocket boosters having the Space Race just being initiated. This accelerated career changes. The first of these involved meeting Professors Earl Parker, Vic Zackay and Gareth Thomas of Berkeley which led to joint papers, involving both basic (2) and applied (3,4) studies for understanding of strengthening mechanisms and toughness of high strength steels. Some of this led to both Ford Scientific Laboratories and Aerojet General in Sacramento given the volatility of the Space Race. This provided access to a new Instrumental technique involving acoustic emission which predicted triangulation to the crack location in the 260-inch diameter booster[5]. This was Thiokol's rocket which failed on the test stand and one of three possible boosters (ours, Thiokol's, and von Braun's) in competition for the moon shot. (If you want an interesting story why we were not successful, give me an e-mail).

Arriving at Berkeley in 1967, an additional opportunity was the investigation of a butterfly spandrel support in the North tower construction of the World Trade Center. See Figure 2. Here, an even more interesting story, which I have not been able to discuss until recently, involved a report sent to the New York Port Authority in the 70s. The third and more scientifically fundamental development concerned metastable austenitic steels. This involved studies initiated at the Ford Scientific Laboratory and completed at Berkeley (3) which produced a combination of high fracture toughness and strength, virtually off the charts(4). Based upon the automotive industry using a lower strength but more inexpensive

version of TRIP (Transformation Induced Plasticity) steel, this led to being named to the *Res Mechanica* Chair at Katholieke, U. in Leuven, Belgium, 2002. Part of this involved presenting seminars at the automotive industry sites which use TRIP steels in current models.



Figure 2: World Trade Center tower being built in 1971. A failed butterfly spandrel support structure was investigated for its future integrity.

II. *The Very Quiet (1970-1980s)*

Taking advantage of the successful application of acoustic emission [5,6], this allowed insight into either alloy additions for improved properties [7-9] or more detailed analysis of one of the two most accepted explanations of hydrogen induced cracking in iron-based systems [10-11]. For brittle fracture, single crystal Fe-3% Si was known to undergo quasi-cleavage fracture. This involved a time-dependent process due to the slow diffusion of trapped hydrogen. In fact, two publications, one in *Acta Materialia* [10] and one in the *Parkins Symposium* volume [11] used acoustic emission events to follow the slow crack growth process. Using the magnitude of two groups and individual emission within the groups, it was concluded that the represented topology required kink advances along the unzipping crack front to be moving at a velocity of 4000 m/s. [11]

III. *The Very Small (1990-2000s)*

Due to the necessity of switching from aluminum to copper lines in conducting electrons between semiconductors, Suo and Hutchinson [12] formulated models for analyzing interfacial fracture of thin films. For finding optimal systems, this required difficult to debond complex interfaces. A series of papers [13,14] solved this problem by proposing a superlayer technique. [13] This produced quantitative interfacial energies as found by others [13] as made possible using a nanoindentation device [14] to better understand thin film deformation. Besides thin films, the yield stress and fracture toughness size effect involving small nanospheres [15], nanopillars [16] and nanocubes [17] was also quantified using *in situ* nanoindentation techniques with SEM and TEM imaging.

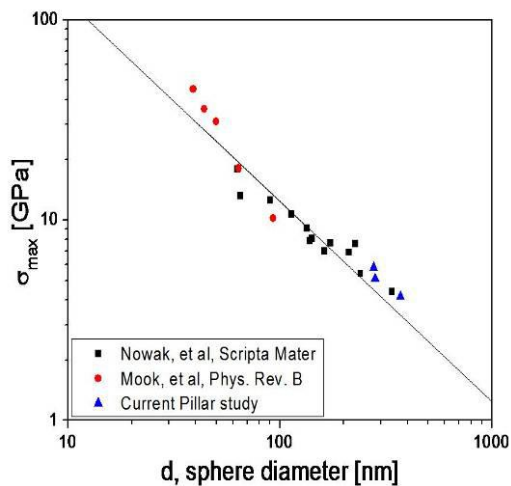


Fig. 3 : Sphere data by Nowak, et al [16] and Mook, et al [15] exhibit a decade increase in strength at small scale. These are comparable to early data by Nowak [16] and others [18]. The three high values for sizes below 50 nm are due to repeat loading with strain hardening which can be modeled by dislocation shielding [19].

IV. Classical Mechanics Weds Atomistic 1990s to 2000s.

With the huge computational capabilities of the newest computers and having a past association with Sandia National Laboratories, [15] it was possible to send a bright and dedicated student [20] to Dr. Jon Zimmerman at SANDIA to facilitate million atom simulations of sphere deformation (See Fig. 4). This produced insightful studies of dislocation emission which eventually led to why the below 50 nm diameter spheres were stronger than expected in Fig. 3. This was based upon dislocation shielding prior to fracture [17,19]. Additional studies involved the indentation size effect [21], nanoindentation simulations [20,21] and the theoretical strength of Si [17,22].

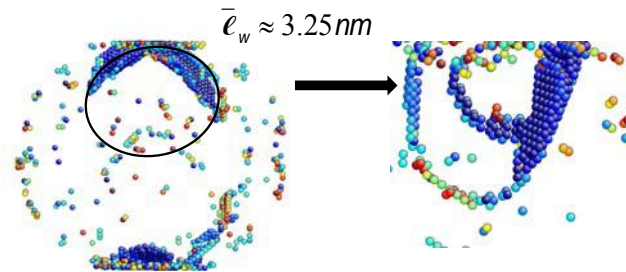


Figure 4. Simulation of 20 nm diameter single crystal silicon with two dislocation loops emitted at the top right having a spacing of 3.2 nm as shown by a rotated orientation.

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Relation Between Structure & Function of the Integral Membrane Proteins

by Etana Padan

Short Biography

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, Rehovot. (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, Federation of the Israeli 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 Garty Regulation 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 commeteete 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

Etana Padan is studying the relation between structure and function of the integral membrane protein NhaA which exchanges Na⁺ for H⁺ across the cytoplasmic membrane of *Escherichia coli*. NhaA and its homologues are essential Na⁺/H⁺ antiporter for pH and Na⁺ homeostasis in enterobacteria and in human cells, respectively. Through Padan’s work NhaA has become a paradigm for this group of membrane proteins. Na⁺/H⁺ antiporters exist in all cell membranes and certain human homologues have long been drug targets because their inactive forms are involved in heart failure and other disorders. Padan’s group cloned the gene from *Escherichia coli*, characterized the antiport activity, over expressed and purified the NhaA protein.

The availability of pure and active NhaA led to join forces with the group of H. Michel (Max-Planck for Biophysics, Frankfurt Germany). H. Michel is a Noble laureate who determined the first crystal structure of an integral membrane protein, the bacterial photosynthetic reaction center. It should be knotted that at that time determining the crystal structure of a membrane protein was a pioneering venture because very few crystal structure of membrane proteins had been solved and no crystal structure of an antiporter existed.

This long standing collaboration is an example of the importance of uniting expertise; Padan in molecular biology, biochemistry/biophysics of antiporters and Michel in structure biology of membrane proteins. Indeed, this collaboration led to the first determination of an atomic structure of an antiporter, a major breakthrough in the antiporters field because the structure has provided key insights into the function and pH regulation of an antiporter, shaded new light on the general architecture of transport proteins and opened the way to structure based interdisciplinary studies that could not have otherwise been applied:

1. Structural insights: The NhaA structural fold is unique; its protein built of 12 helices crosses 12 times the membrane. Two transmembrane segments are unwound and cross each other in the middle of the membrane forming a very delicate electrostatically balanced environment which is essential for the cation exchange activity. Since then, the number of secondary transporters sharing the unique NhaA structural fold, has been steadily increasing, although there is no, or very little, sequence homology between these transporters. Hence, the NhaA structural fold is now recognized as one of the unique folds of secondary transporters.

2. Functional insights: NhaA is a canonical secondary transporter, a “nano machine” that alternates its active site between one side of the membrane and the other. As such, it is highly dynamic and changes its conformation during activity and pH regulation. To understand this mechanism Padan’s group used structural-based approaches, combining computation, structural biology biochemistry, biophysics and molecular biology, and gained the following insights: 1. Elucidating the functional organization of NhaA through site directed mutagenesis and biochemical/biophysical analysis of the mutant’s phenotypes; one group of amino acids forms the active site, another cluster of amino acids participates in sensing the environmental pH and controls the NhaA activity according to intracellular pH. 2. Identifying the pH-induced and substrate-induced site specific conformational changes. This project involved introduction of site specific reporters into the protein. The reporters change their signals upon addition of substrates or a pH shift and report upon conformational changes in specific sites in the protein. 3. Recently, Padan and Michel’s group adopted a MASS spectroscopy technique to follow the global structural dynamics of NhaA. They revealed two sets of ligand-induced concerted movements of helices that have not been seen before. These movements initiate the activation of NhaA. 4. Using the NhaA structure as a template, Padan and colleagues have modeled two important human antiporters: NHE1 a house

keeping human Na⁺/H⁺ antiporter that plays a primary role in heart conditions; and NHA2 the human NhaA ortholog suggested to be an essential factor in essential hypertension. These form first steps toward rational drug design.

We wish to add that before focusing on NhaA, Padan's group discovered anoxygenic photosynthesis in cyanobacteria and photosynthetic bacteria and the responsible integral membrane protein, sulfide quinone-oxido-reductase (SQR). This discovery has been a landmark in understanding the physiology and ecology of photoautotrophic bacteria because until then (1967), the ecology of cyanobacteria was a puzzle: Cyanobacteria, the first organisms responsible for producing oxygen on Earth, were considered to be oxygenic photosynthetic organisms with plant-type photosynthesis although they were found to thrive in anaerobic niches over the globe and drastically polluting many aquatic systems.

This puzzle was solved by the discovery of Padan's group, that cyanobacteria can alternate between oxygenic and anoxygenic- photosynthesis, a property that allow them to dominate and pollute many water sources. Recently, an SQR homologue has been shown to be important in detoxification of sulfide in human.

New Developments in Integrated Computational Materials Engineering (ICME)

by Mark F. Horstemeyer



Short Biography

*Giles Distinguished Professor and CAVS Chair Professor
Center for Advanced Vehicular Systems Chair in Computational Solid Mechanics
Mississippi State University*

Education

PhD 1995 Georgia Institute of Technology, Mechanical Engineering, G.P.A. 4.0/4.0
MS 1987 Ohio State University, Engineering Mechanics, G.P.A. 3.6/4.0
BS 1985 West Virginia University, Mechanical Engineering, G.P.A. 3.7/4.0, Magna Cum Laude

Employment

2015-present Adjunct Professor of Physics, MSU
2013-present Adjunct Professor of Materials Science and Engineering Dept, Tuskegee Univ.
2010-present Honorary Professor of Mechanical Engineering, Xihua University, Chengdu, China
2010-present Adjunct Professor of Agricultural and Biological Engineering, MSU
2009-present Chief Technical Officer, CAVS/MSU
2007-present Founder and Director of Predictive Design Technologies, Inc. (start-up company)
2006-2012 Founder and Director of the DOE Southern Regional Center for Lightweight Designs (SRCLID)
2006-2012 Senior Scientist of DoD Simulation Based Reliability and Safety Center (SimBRS)
2004-present Professor in Computational Engineering, Mississippi State University
2002-present Chair Professor, Mechanical Engineering, Mississippi State University
2002-2008 Sr. Manager, Computational Manufacturing and Design, Center for Advanced Vehicular Systems, Mississippi State University
2002 Manager of Fluid/Thermal Modeling Dept., Sandia National Laboratories, Livermore, CA (15 PhD staff members)
2001-2002 Manager of Chemistry and Materials Process Modeling Dept., Sandia National Laboratories, Livermore, CA (12 PhD staff members)
1999-2001 Principle Member of Technical Staff, Sandia National Laboratories, Livermore, CA
1989-1999 Senior Member of Technical Staff, Sandia National Laboratories, Livermore, CA
1987-1989 Member of Technical Staff, Sandia National Laboratories, Livermore, CA
1986-1987 Engineering Intern, Owens Corning Fiberglas, Granville, OH
1984-1985 Engineering Intern, DOE-METC, Morgantown, WV
1983-1984 Engineering Intern, WV Dept of Highways, Weirton, WV

Honors/Awards:

European Union Academy of Sciences (2017)
Southeastern Universities Research Association (SURA) Scientist of the Year Award-MSU Nominee (2015)
SouthEastern Conference University (SECU) Faculty of the Year Award-MSU Nominee (2015)
American Association for the Advancement of Science (AAAS) Fellow (2013)
Society of Automotive Engineering (SAE) Fellow (2012)
West Virginia University Distinguished Alumni Award (2012)
Giles Professor (Highest Honor at the University), Mississippi State University (2011)

Plasticity Research Award for Young Investigator, Int Conference on Plasticity, Puerto Vallarta, Mexico (2011)
Honorary Professor at Xihua University, Sichuan Province, Chengdu, China (2010)
American Society of Metals (ASM) Fellow (2010)
Thomas French Alumni Achievement Award, Ohio State University (2009)
Ralph Powe Award Mississippi State University (highest university research award) (2008)
ASME Materials Division Chair (2007)
Society of Automotive Engineering (SAE) Teeter Award (2007)
National Leadership Entrepreneurial Award (2007)
American Society of Mechanical Engineering (ASME) Fellow (2006)
Baseball Hall of Fame Physics of Baseball Panel (2004)
Appointed to ASME Materials Executive Board (2004)
Columbia Accident Investigation Board Consultant (2003)
American Foundry Society "Best Paper Award" (2003)
Chair Faculty position MSU (2002)
DOE Recognition Award (2000) USCAR work
R&D100 Award (2000) microstructure-property modeling
American Foundrymen's Society Award (2000) casting modeling
Society of Automotive Engineers (SAE) (1996) technical recognition award
Sandia Doctoral Study Program (1993-1995) internal state variable plasticity
Sandia Award For Excellence (1992) finite element lethality studies
Sandia Award For Excellence (1990) weapons experiments
Sandia Award For Excellence (1989) weapons design

As a fellow of four technical societies (ASME, ASM, SAE, and AAAS), Dr. Mark F. Horstemeyer has garnered national and international acclaim as he has published over 450 journal articles, conference papers, books, and technical reports with a citation impact h-factor of 52 with a total of over 9000 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 150 graduate students and post-doctoral researchers. He has launched 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 a professor in the Mechanical Engineering Department at Mississippi State University (2002-present) holding a Chair position for the Center for Advanced Vehicular Systems (CAVS) in Computational Solid Mechanics, the Chief Technical Officer for CAVS, and Giles Distinguished Professorship at Mississippi State University. Before coming to MSU, Dr. Horstemeyer worked for Sandia National Labs for fifteen years (1987-2002) in the area of multiscale modeling for design.

Dr. Horstemeyer couples multidisciplinary research of solid mechanics, materials, physics, and applied mathematics in three synergistic areas: theoretical multiscale modeling, large scale parallel computational simulations, and chemistry-process-structure-property experimental quantification, which can be summarized as Integrated Computational Materials Engineering (ICME). Dr. Horstemeyer's pedagogical book on ICME (*Integrated Computational Materials Engineering (ICME) for Metals: Reinvigorating Engineering Design with Science*, Wiley Press, 2012) culminated his works for metal alloys. Recently, Dr. Horstemeyer has submitted a follow-on book entitled *Integrated Computational Materials Engineering (ICME): Case Studies*, which focuses on

different horizontal Chemistry-Process-Structure-Property-Performance (CPSPP) examples and vertical multiscale modeling examples that were accomplished for real engineering materials. By employing ICME, Dr. Horstemeyer led a research team that saved 25% weight, increased the load bearing capacity by 50%, increased the fatigue strength by 100%, and decreased the cost from \$15/part to \$13/part of a Cadillac control arm. The notion was that if the whole Cadillac could save 25% weight, then it could achieve 75 MPG, far surpassing the 2025 USA CAFÉ requirements of 50 MPG. Dr. Horstemeyer then employed ICME to redesign the Corvette cradle (C6) by saving 70% weight; this cradle design was employed on the Corvette from 2006 to 2014. Incorporating ICME, Dr. Horstemeyer led another team in saving 12% weight on steel alloy engine bearing caps while ensuring that the load bearing capacity increased 10%. These examples (9 journal articles) not only employed multiscale modeling and experiments but also included multi-objective design optimization methodologies (12 journal articles). The notion in simulation based design is that one can reduce the errors, uncertainties, trial-and-error methods, and costs of engineering products when using high fidelity modeling methods like ICME.

Theoretical multiscale modeling develops and employs techniques that capture structure-properties from the quantum scale to the large structural scale in order to simulate the history of a material in order to predict life cycle performance of structural components. Dr. Horstemeyer coined the phrase “From Atoms to Autos” and has published eight direct literary works that related to ICME. Each of his 450 documents were published in the ICME paradigm, which has been applied to many different areas of materials modeling related to damage/fracture mechanics, plasticity for metals, viscoelasticity for synthetic and biological polymers, geophysical materials, astrophysical materials, and cementitious materials.

Dr. Horstemeyer has published 64 journal articles on damage and fracture mechanics at different length scales, 38 of which were related to studies at the macroscale where he delineated the void/crack nucleation from void/crack growth from void/crack coalescence. He has created an Internal State Variable (ISV) Theory related to damage and fracture that has individual evolutionary rate equations for void/crack nucleation, void/crack growth, and void/crack coalescence, so that the history effects can be captured within a material. Furthermore, these ISVs include subscale morphological features like grain size; particle number density, particle size distributions, particle volume fractions, and particle nearest neighbor distances; and void number density, void size distributions, void volume fractions, and void nearest neighbor distances. As such, each continuum point or element in a finite element mesh can include the multiscale heterogeneities within the mesh. These ISVs are also temperature dependent, strain rate dependent, stress state dependent, and path dependent. They are also generic in the sense that they apply for any metal alloy as Dr. Horstemeyer has applied his damage/fracture theory to over 70 different metal alloys (steel, aluminum, magnesium, titanium, *etc.*). To support the macroscale continuum damage model, studies at subscales were conducted that generated 11 mesoscale journal articles and 6 nanoscale journal articles.

Dr. Horstemeyer is not only a world leader in fracture but in fatigue as well. He has published a total of 38 journal articles on multiscale fatigue, 23 of which were focused on a macroscale MultiStage Fatigue (MSF) model. Similar to the ISV damage/fracture theory, multiscale structures such as grains, particles, voids, *etc.* are included into the MSF model to predict a more accurate lifetime. In the MSF model, several mathematical terms are

included that represent different physical realities of the fatigue process. Historically, fatigue had been denoted at initiation and propagation, where propagation started at about 250 microns in size, because we could not see the cracks below that size with our naked eye. "Initiation" was defined as everything before propagation. Since the advent of microscopy, we have the capability of examining lower length scale mechanisms and phenomena. What Dr. Horstemeyer realized was that there was an incubation, or pregnancy period, before a crack started. Furthermore, other researchers had defined a Microstructurally Small Crack (MSC) regime, where the microstructural details played a very large role in determining the crack path. As such, Dr. Horstemeyer along with his colleague Dr. David McDowell suggested that there exists multiple stages in fatigue: incubation, microstructurally dependent crack growth, and then Long Crack (LC) growth, which relates to the old term of propagation. Hence, for multiscale structures embedded within a material system, the MSF model predicts a different number of cycles for incubation, MSC, and LC regimes. The finite element with the lowest total cycles will be the failure location. Hence, the MSF model predicts the fatigue life of a complex metal alloy in any region of a complex engineered part. Similar to the ISV damage/fracture model, the MSF model is generic and has been applied to several steel, aluminum, magnesium, and titanium alloys. To support the macroscale MSF model, studies at subscales were conducted that generated 9 mesoscale journal articles and 6 nanoscale journal articles. Finally, Dr. Horstemeyer was the first to run atomistic simulations on fatigue and developed the term "Nanostructurally Small Cracks."

Fracture and fatigue are not the only inelastic materials' behaviors that Dr. Horstemeyer has studied, but in fact he has published 77 journal articles on plasticity as well. Regarding plasticity he has published 18 journal articles at the macroscale employing ISVs that represent the effects of isotropic and anisotropic dislocation behaviors, 27 journal articles at the mesoscale that mainly focused on crystal plasticity and texture modeling and experiments, 4 dislocation dynamics journal articles, and 28 atomistic plasticity related articles. He and his colleague Dr. Mike Baskes, the father of the Embedded Atom Method (EAM) and Modified Embedded Atom Method (MEAM) potentials, were the first to study plasticity employing computational atomistic methods. One particular insight that they found was that the yield strength of a material increased six orders of magnitude as the length scale (volume per surface area) parameter decreased ten (2?) orders of magnitude (Horstemeyer, M.F., Plimpton, S.J., and Baskes, M.I., "Size Scale and Strain Rate Effects on Yield and Plasticity of Metals," *Acta Mater.*, Vol. 49, pp. 4363-4374, 2001.) This volume-per-surface-area related to yield strength assertion was shortly experimentally validated (Gerberich, W.W., Tymak, N.I., Grunlan, J.C., Horstemeyer, M.F., and Baskes, M.I., "Interpretations of Indentation Size Effects," *J. Applied Mechanics*, Vol. 69, No. 4, pp. 443-452, 2002.).

Associated with the multiscale modeling and CPSPP sequence modeling that was mentioned in the previous paragraphs, Dr. Horstemeyer has been involved in modeling and simulating different materials processing methods (59 journal articles) that include the following: casting (27 journal articles), forming/rolling/extrusion (16 journal articles), powder metallurgy (17 journal articles), welding (9 journal articles), Laser Engineered Net Shaping (LENS) (3 journal articles), machining (2 journal articles), galvanizing (1 journal article), and springback (1 journal article).

The aforementioned studies have focused on complex thermomechanical couplings in the CPSPP sequence. Recently, Dr. Horstemeyer added chemistry into the multiscale thermomechanical plasticity-damage theory in terms of hydrogen embrittlement and corrosion (14 journal articles). Currently, 8 different journal articles have focused on the development of the macroscale ISV theory that adds general corrosion, pitting corrosion (three separate ISVs for nucleation, growth, and coalescence), and intergranular corrosion and the associated experiments that were used to calibrate the model. The mesoscale analysis included 2 journal articles and the nanoscale included 4 journal articles, all of which fed into the macroscale modeling.

The focus of the preceding work has been on metals, but Dr. Horstemeyer has extended the ICME paradigm to synthetic and natural polymers as well (46 journal articles). For synthetic polymers (13 journal articles), the same multiscale modeling of inelasticity with the use of damage ISVs has been employed at the macroscale (7 journal articles) with subscale information (1 mesoscale journal article and 5 nanoscale journal articles) feeding into the macroscale model. Based upon this multiscale polymer modeling, composites modeling has arisen (4 macroscale journal articles, 2 mesoscale journal articles, and 2 nanoscale journal articles). Also, based upon the multiscale polymer modeling, biological (25 journal articles) materials modeling and experimentation has been able to grow at the macroscale (23 journal articles) and at the nanoscale (2 journal articles). The ICME paradigm has allowed analysis of porcine brain, woodpecker beaks, ram horns, turtle shells, armadillo shells, and rabbit tendons. These studies have helped create a paradigm for bio-inspired design related to impact mechanics and for simulating the human as well within impacts such as car crashes and sports helmets.

Other areas of research that Dr. Horstemeyer has recently employed the ICME paradigm has been in the areas of geodynamics (4 journal articles), astrophysics (1 journal article), and cementitious materials (1 journal article). These areas along with some other multiphysics areas are a focus for future growth, where multiscale modeling can provide great scientific insights.

Innovative Construction Research Projects

by Behrokh Khoshnevis

Short Biography

Academic Experience

2005-present Director, Center for Rapid Automated Fabrication Technologies (CRAFT)

1997-present Professor of Industrial & Systems Engineering, and Director of Manufacturing Engineering Graduate Program (since 1992) University of Southern California.

1987-1997 Associate Professor of Industrial and Systems Engineering, and Associate Director of Manufacturing Engineering Program (1984-1992), University of Southern California.

1983-1987 Assistant Professor of Industrial and Systems Engineering, University of Southern California.

1980-1983 Assistant Professor of Industrial and Systems Engineering, Ohio University.

1979-1980 Visiting Assistant Professor of Industrial Engineering and Management, Oklahoma State University.

Professional Affiliations

National Academy of Inventors, Fellow

European Union Academy of Sciences, Member

Institute of Industrial Engineers, Fellow

- Chairman, Academic and Research Committee on IE in Construction, 2003-present

- USC IIE Student Chapter Faculty Advisor, 1984-1990

- Chairman of IIE Manufacturing Division for Region XII, 1985-86

- Chairman of IIE Production and Inventory Control Division for Region XII, 1984-85

- Conference Chairman, IIE Los Angeles Chapter Conference, March 1984

Society for Computer Simulation, Fellow

- Member of Board of Directors, 1994-5

- Member and past Chairman of Steering Committee, Western Simulation Council, 1991-2002

Society of Manufacturing Engineers, Senior Member

American Association for Advancement of Science (AAAS), Member

Standing Member of the Emerging Technology Committee, Infrastructure Resilience Division, American Society of Civil Engineering (ASCE)

Learning International Network Consortium (LINC), Member of Advisory Board

Sharif University of Technology Association (SUTA), Member of Scientific Advisory Board

Association of Professors and Scholars of Iranian Heritage, Member of Advisory Board

Editorial Boards

Member of Editorial Board of: *Journal of 3D Printing and Additive Manufacturing*, *Int. journal of Rapid Manufacturing*, *Journal of Intelligent Manufacturing*, *Int. Journal of Industrial & Systems Engineering*, *Journal of Computers & Industrial Engineering*, and *Journal of Industrial & Systems Engineering*. Guest Editor of *Journal of Automation in Construction on Large Scale 3D Printing*.

Awards & Recognitions

1. Khwarizmi International Award recipient (KIA Laureate), 2016
2. Elected as Member, European Union Academy of Sciences, 2015
3. Hall of Fame Inductee, Oklahoma State University College of Engineering and Architecture, 2015
4. 3D Printing World Award, Mumbai, 2015
5. Best Paper Award, 2015 Solid Free Form Fabrication Symposium
6. Received the Orange County Engineering Council Distinguished Engineering Merit Award, February 2015.
7. Appointed as Dean's Professor at USC in December 2014.
8. Inducted as Fellow of the National Academy of Inventors in 2014.
9. Recipient of the Grand Prize (as the top among 1000+ globally competing technologies) of the NASA Creating the Future design contest for invention of the Contour Crafting robotic construction technology. The program is sponsored by Intel, HP and several other major industries.
10. Best Paper Award, 2014 Solid Free Form Symposium.
11. Best of 2014 Papers, special issue of 3D Printing and Additive Manufacturing
12. Selected as one of only two US university faculty to present research project at Capitol Hill on NASA Technology Day 2013
13. Best Paper Award by ISA PMCD - 58th International Instrumentation Symposium, 2013

14. TEDx presentation on automated construction has been ranked by the TED organization as one of top five among more than 30,000 TEDx talks and has been viewed over a million times (as of Dec 2013) and counting (see the TEDx talk at www.ContourCrafting.org)
15. Creative-Iran Society Gold Trophy Award 2012
16. Sharif University Alumni Achievement Award, 2012
17. Awarded Fellow status, NASA Innovative Advanced Concept (NIAC), 2011
18. Winner of Innovation in Curriculum Completion Runner-up, Institute of Industrial Engineering, 2008
19. Automated construction invention selected as one of top 25 inventions among 4300 contestants by The National Inventor's Hall of Fame, History Channel Modern Marvels program, and Time Magazine, 2006
20. USC School of Engineering Senior Research Award, 2005
21. 2005 Pete Lohmann Medal (Best OSU Engineering Alumni)
22. Awarded Fellow of the Society for Computer Simulation, 2004
23. Technical Innovation in Industrial Engineering Award, Institute of Industrial Engineering, 2004
24. Highest Honor Award for Innovation in Construction, Construction Specification Institute, Gulf State Region, 2004
25. Best Paper Award, selected by Emerald Publisher's Rapid Prototyping Journal Editorial Board, 2004
26. Outstanding Scholar Award, Association of Professors and Scholars of Iranian Heritage, 2004
27. Best Paper Award, 19th International Symposium on Automation and Robotics in Construction, 2002
28. Best Paper Award, Solid Free Form Symposium, 2002
29. Awarded Fellow of the Institute of Industrial Engineers, 1999
30. Member of Alpha Pi Mu, Omega Rho, and Tau Beta Pi Honorary Societies
31. Contour Crafting has been exhibited at numerous science as well as art museums worldwide

Contour Crafting Simulation Plan for Lunar Settlement Infrastructure Build-Up

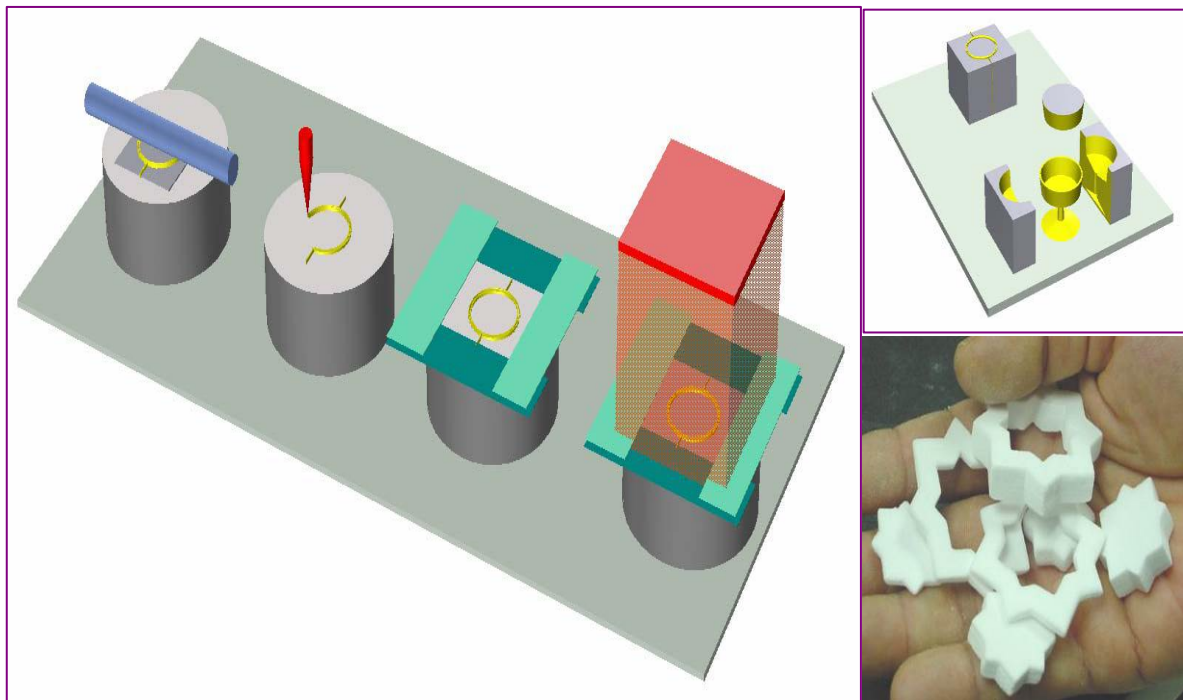
Source: NASA

Economically viable and reliable building systems and tool sets are being sought, examined and tested for extraterrestrial habitat and infrastructure buildup. This NASA NIAC project utilizes a unique architecture weaving the Contour Crafting automated building technology with designs for assisting rapid buildup of an initial operational capability lunar base. Using the CC technology, this project intends to draw up a detailed plan for a high fidelity simulation at NASA's D-RATS facility, to construct certain crucial infrastructure elements in order to evaluate the merits, limitations and feasibility of adapting and using the CC technology for extraterrestrial application. Elements suggested to be built and tested include roads, landing pads and aprons, shade walls, dust barriers, thermal and micrometeorite protection shields and dust-free platforms as well as other built up structures utilizing the well known in-situ-resource utilization (ISRU) strategy.



Selective Inhibition of Sintering – SIS**Source: NSF**

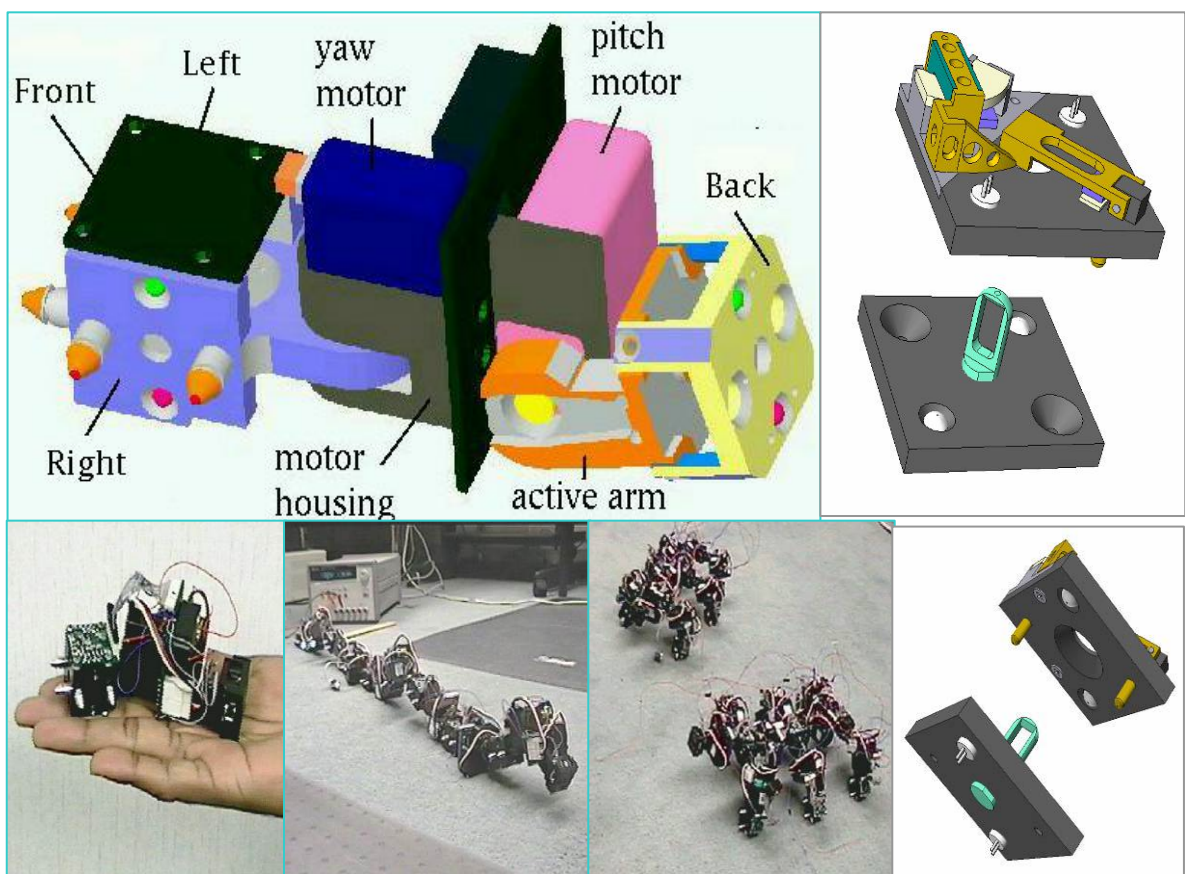
SIS is a solid free form fabrication process which has been invented at USC. SIS builds 3D objects in a layer wise fashion using powder sintering. Addition of an inhibitor liquid to part section profiles on each powder layer inhibits the sintering of affected powder particles under a radiative heat. An Alpha machine has been designed and developed and numerous experiments have been performed under this grant and various parts have been built out of various polymeric as well as metallic materials. The PhD dissertation by Dr. Bahram Asiabanpour contains the details of the study.



Docking System for Self Reconfigurable Robots (PIs: Dr. Peter Will & Dr. Wei-Min Shen)

Source: DARPA

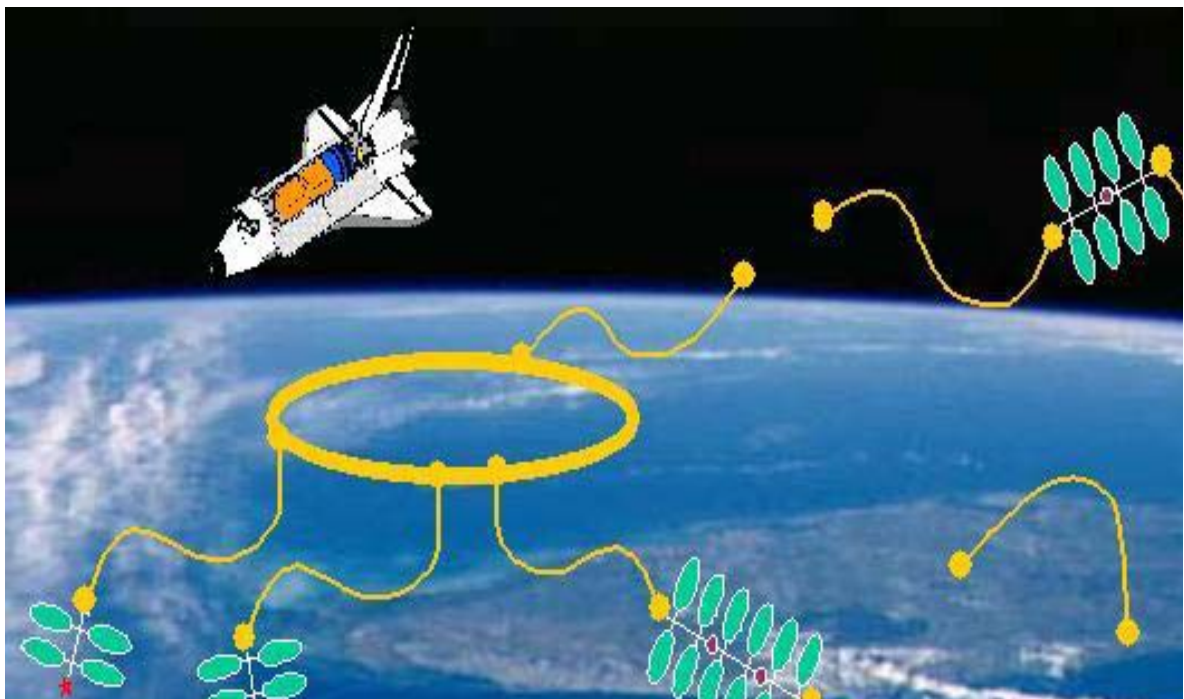
A new docking system called *Compliant-And-Self-Tightening* (CAST) is developed as an effective and efficient connector for joining and releasing modules of self-reconfigurable or metamorphic robotic systems. CAST has been successfully implemented in CONRO (see www.isi.conro) where its highly compliant and passive features have allowed a considerable ease of execution of a variety of docking algorithms, while using no additional energy for docking and negligible amount of energy for undocking. Development of CAST was motivated by observing the difficulty of implementation of an earlier less compliant docking system.



Space Reconfigurable Robotics Assembly System (with Dr. Wei-Min Shen & Dr. Peter Will)

Source: NSF

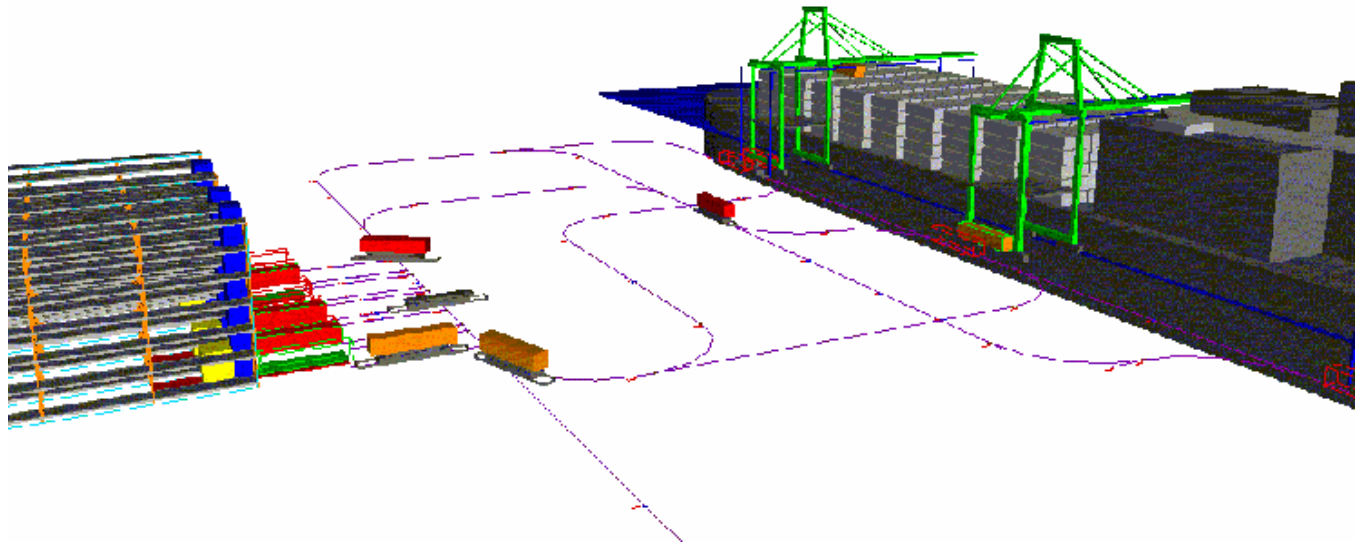
This project concerns the autonomous assembly of space solar panels using cable-connected robotics modules that are capable of compliant docking to assembly components and pulling them to the desired location. The project has used an air table for testing a physical simulator system in a 2D space.



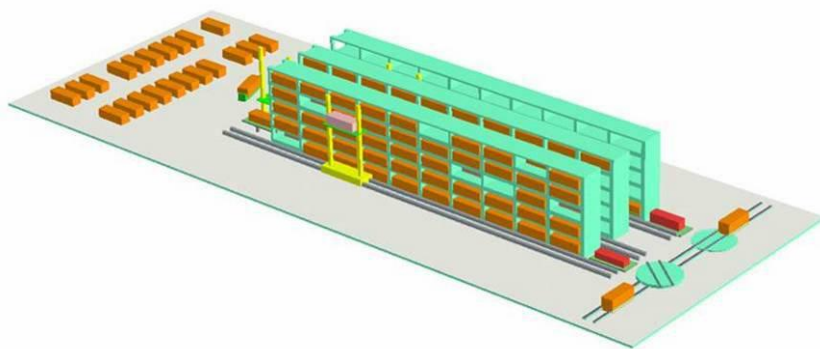
Automation of Material Handling and Storage at Marine Terminals

Source: METRANS

This project concerns systematic analysis and design of port terminals using physical and virtual computer simulation, and evaluation of automated material handling and storage systems for timely handling of containers at ports. Virtual and physical models of AGV and AS/RS systems are built to evaluate various effects and identify certain parameters for efficient and effective modern port systems.

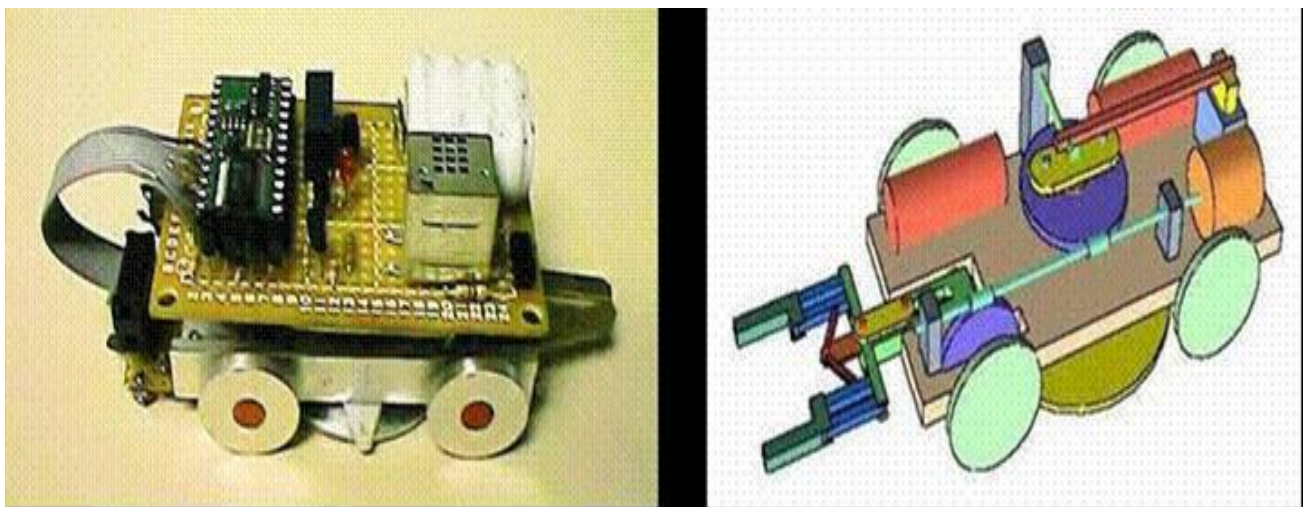


A 3D view of the yard layout and the simulation model



Multiple Mobile Robots in Manufacturing Assembly (Co-PI: Dr. George Bekey)
Source: NSF

In this project the development of a new system of supervision, sensing, control, and intelligence, for a colony of robots, organized for the performance of specific tasks have been investigated. As compared to local sensing and control the new approach could offer many advantages. Various hardware systems as well as planning and control software have been developed for this project. Low precision manufacturing assembly has been the focus of the experimentations involved in



Far Ahead of His Time – The Universal Scholar Gottfried Wilhelm Leibniz (1646 – 1716)

by Erwin Stein, Member EUAS



Short Biography

Univ.-Prof. em. Dr.-Ing. habil. Dr.-Ing. E.h. Dr. h.c. mult.

Institute of Mechanics and Computational Mechanics

Leibniz Universität Hannover, Germany

Studies of Civil Engineering and Mathematics at Polytechnical University of Darmstadt, Germany, Construction and Analysis of wide-spanned Bridges in industry, Promotion and venia legend at the University of Stuttgart, Ordinarius of the Chair of Mechanics and Computational Mechanics of the University of Hannover, Official Inspection Engineer for Structural Engineering in the Land of Lower Saxony

*Founder and Curator of the Leibniz exhibitions of the Leibniz Universität Hannover
Honorable Doctor of the Universities of St. Petersburg, Stuttgart, Xuzhou/Beijing and Poznan*

Gauß-Newton Congress Medal of IACM, Zienkiewicz Medal of the Polish Ass. For Computational Mechanics (PACM), Ritz-Galerkin Medal of ECOMAS, Awarding with the Verdienstkreuz 1. Klasse des Niedersächsischen Verdienstordens

Honorable-Member of IACM and GAMM

Member of several Academies of Sciences in Germany and Europe

Editorial board-member of 8 international scientific journals

Lead editor of the Encyclopedia of Computational Mechanics (ECM), forthcoming 2nd electronic edition

425 scientific publications (including 16 books as author, co-author, editor, and/or co-editor) on kinematic, material, and mathematical modeling of technical objects together with computational mechanics, i.e. computer-oriented numerical methods (esp. finite element methods), error analysis and adaptivity, algorithms, and software engineering in continuum and structural mechanics, and application to complex engineering problems. Principal editor of the "Encyclopedia of Computational Mechanics" with 3 volumes consisting of 75 articles on approx. 3.000 pages, published by John Wiley & Sons, Chichester, UK, and also available on the Internet since October 2004. First electronic revision in 2007. Forthcoming second electronic edition in 2016.

Co-editor and member of the Editing Boards of 8 national and international scientific journals 51 DFG research projects, including "Special Research Areas", chairman of "Priority Projects" within Germany, chairman of "Priority Projects" at the University of Hannover and individual research projects.

4 joined research projects, supported by the Volkswagen Foundation, Hannover

Several industrial research projects, mostly concerning the evaluation of damage and failure

Initiation and supervision of 54 doctor theses of students at our Institute and reviews of 30 further doctor theses

Initiation and reviews of 9 habilitation theses of institute members and 4 further habilitation theses at

other universities

As a result of nearly 30 years of establishing a school of Computational Mechanics as a new important subject at the Leibniz Universität Hannover, 10 former members of the institute became full professors (with chairs) at German universities, and 13 former members became professors at universities of applied sciences (Fachhochschulen)

1. Introductory Remarks

G.W. Leibniz, born 1646 in Leipzig lived and worked in Hannover for 40 years as a councilor to the dukes and later the elector until his death in 1716. Next to Descartes, he was a leading philosopher, mathematician, scientist, and technical inventor at the beginning of the age of enlightenment. He is said to have been the last universal scholar, with the belief that all is connected to everything. His new ideas, achievements, and inventions were far ahead of his time, especially philosophically, with his theory of science, the infinitesimal calculus and the invention of decimal and binary calculating machines.

Since 1990, I conceived and realized the travelling Leibniz Exhibition of our university, presented eleven times in Germany and Austria, with the slogan *Leibniz to Grasp and Understand*, which became a permanent exhibition at our university since 2008. It includes about 30 replicas and functional models of the decimal and binary calculators, the cyphering machine, models for the Brachistochrone Problem (the curve of shortest time for a downwards gliding or rolling mass), marking the beginning of variational calculus. Replicas and models of his inventions for silver mining in the Harz mountains and the Herrenhausen water fountains are also part of the exhibition.

All these ideas and inventions follow his postulates *Theoria cum praxi* (theory integrated with practice) and *Bonum commune* (for the common good).

From our experience of many lectures and exhibition guides, not only people with a degree, but many other people are interested in experiencing Leibniz. A further intention of this contribution is the experience that Leibniz is fairly unknown outside of Europe, e.g. in the United States; where he is overshadowed by Isaac Newton in the fields of mechanics and mathematics. I believe that Leibniz further merits international recognition according to his important and far-reaching theoretical and practical contributions, still with a strong influence present in today's philosophy, science, and technology.

2. Leibniz' Maxims of Thinking

- (1) *Nihil sine ratione; Nihil fit sine causa sufficiente*, the causality principle
- (2) Theorem of Identity and Contradiction; all that exists, exists, and cannot be and not be in the same time and place.
The maxims (1) and (2) were already postulated by Aristoteles.
- (3) Leibniz' Theorem of the Identity of the Indistinguishable; two different things cannot have all their properties in common. This theorem was criticized in quantum mechanics but is of interest in today's theoretical physics of the macro- and microcosms, trying to generalize and unify the theory of relativity with quantum mechanics based on generalized String-theory, mathematically based on algebraic geometry.
- (4) Continuity Principle, *natura non facit saltus*

3. Leibniz' Program for the Theory of Science

Based on the Aristotelian syllogistics for the foundation of logics and following his fundamental goals and ambitions for the development of science and technical inventions, Leibniz set up the following branches of universal science:

- (1) *Scientia generalis*, a general deductive and deterministic or probabilistic logic of science with new structural concepts for all disciplines with the postulate, *Theoria cum praxi*;
- (2) *Characteristica universalis*, the invention of suitable signs and systems and their connections to formulas for a logically sound and universal language of science for the analysis and synthesis and also for the colloquial day-to-day language.
- (3) *Ars inveniendi*, in connection with the *Ars combinatoria*, the art of inventing technical products and systems by a synthesis of facts and relations, gained by the analysis and exclusionary criteria, using the *Ars combinatoria*

- (4) *Calculus logicus*, based on the four Aristotelian forms of syllogistics: universally or partially affirmative as well as universally or partially negative. Leibniz developed an incomplete system of set-theoretical definitions and 51 theorems, first published only by Franz Schupp by Meiner-Verlag, (2000), wherein Leibniz anticipated a considerable part of George Boole's book, *The Mathematical Analysis of Logic* (1847). It should be remarked that most of the technical norms and legal texts are formulated in colloquial language with many logical contradictions, especially concerning contradictions between commandment and prohibition as well as between permission and exemption.

4. Leibniz' Philosophy-- The Monadology: Science and Metaphysics

From logical point of view, it has mathematical structures, see his statement: *my metaphysics could well become mathematics*. The most important writings are: *Discours de Métaphysique* (1686), *Système nouveau de la nature* (1695), the *Theodizée sur la Bonté de Dieu, la Liberté des Hommes et l'origine du Mal* (1710), and the *Monadology* in French (1714), German translation (1720).

The Greek word *monas* means unity; the monadology has 90 paragraphs, briefly summarized with the terms, perspectives and interior structures of his metaphysics as a counter draft to Descartes' purely mechanistic philosophy, published in the *Discours de la méthode* (1637) being the spectacular dawn of the age of enlightenment. The cornerstones of Leibniz's *Monadology* are:

- (1) A Monad is a God-created simple, indivisible mental substance, bound to a living being, as part of its identity (§1);
- (2) Monads do not have windows (§7); they are self-sufficient and unmistakable, but they necessarily possess a so-called pre-established harmony for conflict-free, empathic, mutually beneficial coexistence in their love towards God and man.
- (3) Outer *perceptions* of the senses are transferred to the complete state of a monad and reflected with others in harmony. Monads should strive to higher perceptions accompanied by consciousness and reflexive recognition, called *apperceptions*.
- (4) God's expectation of the monads is moral fulfillment.
- (5) The unity of God and human souls is a solution to the important "body-soul" problem, which is not possible on Descartes' mechanistic philosophy.
- (6) The monads underlie the principles of change and of the diversity in unity (§§13, 14).
- (7) Leibniz combines the universal harmony of Greek philosophy with the new individual harmony of the monads.

5. Immanuel Kant's Critiques on Leibniz' Intellectual System of the World and late Justification

Kant did not accept Leibniz' holistic metaphysical-scientific world as the best of all possible worlds: *Monads were inventions of the mind to explain the world without having understood it, because the experience of reality would be missing. Leibniz would not have given a specific kind view towards sensuality. His concept was the confusion of the pure object of mind with its appearance.*

Leibniz' late justification: He strictly decides between *the appearances* (according to Kant's transcendental philosophy) *and the theoretical constructions based on them. This is also today's mathematical modelling in science and the solutions for real states and processes and thus the logically sound representation with a relative truth, limited only by time*, which is also the methodology of today's research. Our mathematical, scientific, and applied current goals are therefore *verification and validation*.

6. Mathematics – Infinitesimal Calculus, Determinants

Infinitesimal Calculus Leibniz independently discovered the infinitesimal calculus (differentiation and – inverse – integration) independently from Newton in the early 1670s in Paris, about 3½ years after Newton. His originality was only confirmed in 1947 by a mixed English-German mathematical commission, after a long period of accusing Leibniz of plagiarism until his death. In the historical sequence of Archimedes, Kepler, Galilei, Cavalieri, Wallis, Fermat, Barrow and especially Newton and Leibniz. This calculus became the basis for modeling and analysis in science, technology and in humanities. Leibniz' calculus was published in 1684 [1] and Newton's only in [2] (1687). It should be mentioned that Leibniz got his inspiration by an article of Blaise Pascal from 1658 where he presented the $\tan \alpha$ of the tangent of a circle

which in this unique case is given by the quotient of two finite coordinate increments. Leibniz' infinitesimal calculus is much deeper and broader than Newton's, with, e.g.: (1) chain-, product- and quotient rules, power series for $\arctan \pi/4$, methodus tangentium inversum, partial derivatives of functions depending from several variables, integration of differential equations, funicular curves in different representations, geometric integration of the differential equation of the common cycloid as well as proving the integrability of functions in a sequence of finite steps by using already Riemann sums from the 19th century.

Determinants Leibniz learned combinatorics from Prof. Erhard Weigel in Jena, 1663 which remained challenging for his whole life. He used them for the evaluation of polynomials with single and double indices, the conversion of power series and especially for the solution of systems of algebraic equations and related eigenvalue problems for which he used the terminology and theorems of determinants, published in [3] (1700). In his article [4] (1710) he introduced a new terminology (*novum designationis genus*) with double indices for two quadratic algebraic equations with a representation near to Sylvester's matrix notation from the 19th century. Leibniz also anticipated the so-called Gabriel Cramer's rule for the solution of linear algebraic equation systems (1750).

Historical Remarks: the roots of determinants can be traced back to Chinese mathematics in the early Han Dynasty (202 BCE and 9 AD), with linear algebraic equation solvers in the 9 books of arithmetic techniques, the *Chiu Chang Suan Shu*. At the same time as Leibniz the determinant calculus was discovered by Tabakazu Seki in Japan which he called *Kaifuku-dai no Hō* (Method for solving *fukudai* problems), for, e.g., the elimination of a common variable from two equations of higher order.

7. Mechanics – The True Measure of the Living Force

The development and the quarrels about this important issue required nearly a century, and were only finished by Isaac Newton in his millennium work, the *Principia* [5] (1687) which established classical mechanics and modern natural science. Integration in time of his fundamental law of dynamics,

$$F(t,s) = m \cdot \frac{dv(t,s)}{dt}$$

, yields the impulse theorem, and integration in space the energy theorem. Adding the potential energy of a mass, one gets the conservation principle of total energy. Descartes had presented 7 theorems for the impact of two bodies based on the conservation of $m \cdot |v|$, first not regarding that the nominal value of vector v has to be used. [6] (1637). Leibniz detected that these so-called laws were wrong, and published his *True Measure* in [7] (1686), namely the kinetic energy

$$K = \frac{1}{2} m v \cdot v$$

, using Galilei's result for the velocity of a falling mass in the gravity field g , $v = \sqrt{2gh}$ in [8] (1638); Leibniz did not include the factor $\frac{1}{2}$, and his formula is only valid for quasi-static movements of mass.

8. Mathematics – Begin of Variational Calculus and Optimization Problems in Mechanics

The first minimal principle of rigid body mechanics was published by Torricelli (1630), secretary to Galileo Galilei, stating that the gravity center of static force systems (e.g. due to gravity loads) takes its deepest possible position in stable static equilibrium, which is the principle of minimum potential energy. Then in 1675 Fermat discovered that the path taken by light between two fluids of different densities takes the shortest possible time, not the shortest way, based on Snellius' reflection law from 1621. Galilei published his experimental results of a frictionless downwards gliding mass on a skew plane, and then on polygons with an increasing number of vertices for which the gliding time decreased. He proposed a circular arc as an approximate analytical solution [8] (1638).

Johann Bernoulli published a call for an analytical solution of this so-called *Brachistochrone problem* in one year's time in [9] (1696). 7 solutions were submitted, until spring of 1697, published by Leibniz in *Acta Eruditorum*, [10] (1697). The most important one is the first analytical solution of this problem, by his older brother Jacob Bernoulli with the idea to formulate this problem first by n discrete problems at equidistant nodal points at coordinates $y_i - h$, y_i and $y_i + h$; $i = 1, 2, \dots, n$, of the descending curve with triangular test and trial functions between 3 points, respectively, Fig. 1.



Jakob Bernoulli, 1655-1705

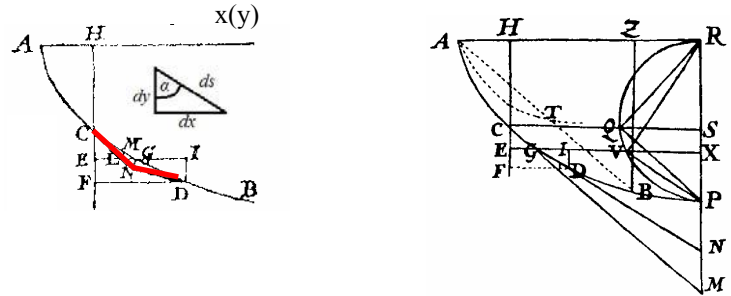


Figure 1: Jacob Bernoulli’s analytical solution of the Brachistochrone problem, based on a discrete modeling with triangular test functions, anticipating Leonhard Euler’s solution from 1736

With the discrete stationarity condition $\delta_{CD} + \delta_{CB} = \delta_{CA} + \delta_{AB}$ of the extremal problem the continuous limit $h \rightarrow 0$ yields the differential equation of the extremal function, which is the common

cycloid, resulting in $\frac{ds}{dx} = \frac{k}{\sqrt{y}}$ and $\tan \alpha = \frac{dx}{ds} = \sqrt{\frac{y}{k^2 - y}}$ with $k^2 = 2r$, with α as the rolling angle. The parametric representation of the cycloid follows as $x = r(\alpha - \sin \alpha)$; $y = r(1 - \cos \alpha)$.

Leonhard Euler published the generalization to isoperimetric problems in 1743, using the same idea as Bernoulli of starting with a sequence of discrete points of the optimal curve. As well known, using this discrete derivation is troublesome for the second variation. Therefore Lagrange’s method using the embedding ansatz $x(y) = x_0(y) + \epsilon \eta(y)$, x_0 being the extremal function, is used since thereafter.

Leibniz proposed two solutions, the first as the exact piecewise geometric integration of the differential equation of the cycloid, and – even more interesting – the second one as the geometrically presented concept for the direct (or discrete) numerical solution of the Brachistochrone problem using the same equidistant nodal points and triangular test and trial functions as in Jakob Bernoulli’s analytical derivation published in Leibniz’s article from July 1697 in *Acta Eruditorum*, fig. 2. Leibniz did not present the discrete variational calculus, leaning to a system of nonlinear algebraic equations for the coordinates of the nodal points, despite the requests of Johann Bernoulli. This analysis was published by E. Stein and K. Wiechmann [11] (2004), which proves Leibniz to be the first predecessor of the Finite Element Method (FEM), see also E. Stein [12] (2014)

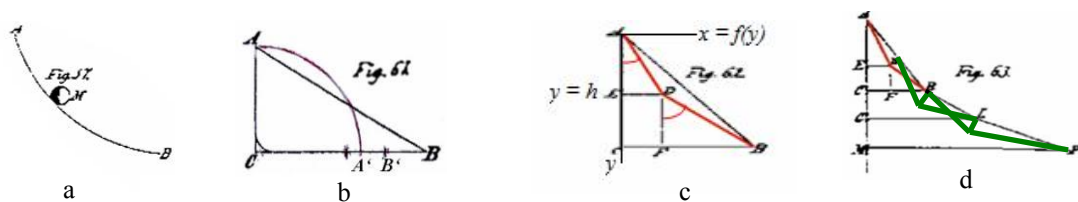


Figure 2: Leibniz’ geometrical draft of a direct variational calculus for the Brachistochrone problem; 2b: restriction of the solution area; 2c: triangular test and trial functions between 3 equidistant nodal points with one unknown coordinate of the gliding curve at $y = h$; 2d: the same technique for 5 nodal points 3 unknown coordinates, first published by G.W. Leibniz in *Acta Eruditorum* July 1697.

The stationarity conditions for minimal time yield a system of nonlinear algebraic equations at the nodal points.

9. Leibniz’ Decimal Four-Species Mechanical Calculators

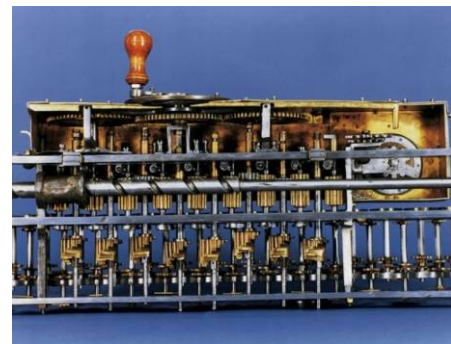
Leibniz had realized that the quickly developing mathematics and science, especially astronomy, required four-species calculators with many digits, extending beyond addition and subtraction as in Blaise Pascal’s *Pascaline* from 1650. Leibniz tried to implement this extension by adding an additional component but

obviously could not realize this together with Antoine Ollivier, a distinct Parisian watchmaker in the years between 1672 and 1676. Adding two 6-digit numbers with the *Pascaline* required the user to sequentially rotate the six input gears with a stylus from the desired digits counterclockwise to 0, followed by adding the next number in the same fashion. The decimal carries are executed correctly due to the sequential input of all digits. After constructing the machine, Pascal was asked by his father, a tax collector, to also provide a subtraction operation which was ingeniously implemented by using complementary digits, marked in red, but it is not difficult to realize subtraction in Pascal's machine with a spring-mounted – in place of a gravity-operated – lever.

Consequently, Leibniz designed a new numerical input where the complete multiplicand (with all digits) is entered into the input carriage, and then transferred at the same time as a whole by a rotation of 360° of the *Magna Rota* crank, so that all digits are added simultaneously into the calculating unit. All further numbers are entered in the same way in different places along the input carriage, according to the rules of numbers, given here in the decimal positional notation, fig. 3. This figure shows the only remaining original so-called “younger large four-species mechanic calculator” with 8 input places, 16 result places, and 1 counting place. It was built in between the late 1690s and early 1700s in Helmstedt and improved in Zeitz, Saxony, and brought back to Hannover shortly before Leibniz' death in November 1716.



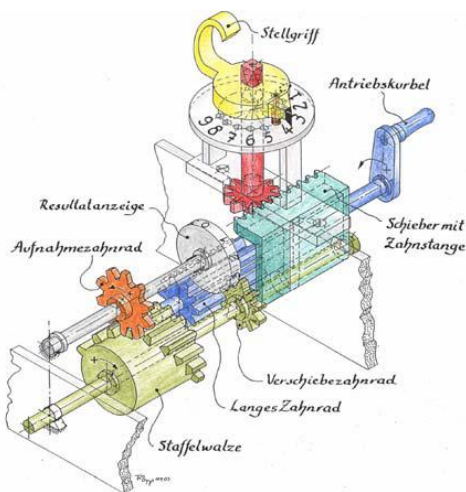
a



b

Figure 3a: Leibniz' younger decimal four-species calculator (front view) with two main function groups (the input carriage with 8 input digits, the *Magna Rota* crank in front and the carriage shift crank on the left hand side), the rotation counter at the upper right of the carriage, and the calculating unit itself in the back; 3b: view of the machine from below, with 8 stepped drums (for 8 digit inputs) which are actually moved by individual gear racks. In the upper part of the figure we see the *Magna Rota* crank with the distribution of the rotational moment onto 3 input gears in order to minimize the margin of error due to manufacturing inaccuracies.

Figure 4 demonstrates the construction of the input of a digit via the stepped drum, an original invention by Leibniz.



a



b

Figure 4a: perspective of a digit input via the stepped drum, axially moved with a pinion (Zahnstange) by the input handle (Stellgriff) such that the desired number of gear teeth are beneath the recording wheel (Aufnahmezahnrad), such that rotating the *Magna Rota* crank (Antriebskurbel) rotates the pickup gear by the desired number of digits; its shaft transfers this number into the calculating unit.

The most important, complicated, but very efficient part of Leibniz' machine is the construction of decimal carriers, figure 5, which functions as follows: rotating recording wheel from 9 to 0 initiates the first part of the decimal carry by rotating the five-bay-wheel with the one-toothed gear (on the shaft of the pickup gear) by 18° ($=36/2$). At the shaft of the five-bay-wheel is the five-horned wheel with a pre-rotation of 18° ; then this wheel enters the orbit of the twin-horn, which, by rotating the *Magna Rota* crank, rotates the five-horn wheels – in this second part of the decimal carry – by a further 36° , in total $72^\circ=360/5$ according to the five horns of five-bay-wheel and the five-horn-wheel; it must be an odd number of horns, because only the next left counting (or result) wheel should be rotated by 36° in case of a decimal carry, but only 21.5° are rotated by pure kinematic rotations, such that the remaining 14.5° are forcefully rotated by the dwelt notch wheel (Rastkerbenrad) actuated by flange pressures of a spring-mounted wheel and an additional spring-mounted wheel acting on the results wheel directly.

As explained above, decimal carries may not be completed. This is indicated at the related place by a pentagon disk (Pentagonscheibe) at the end of the decimal carry shaft, which is rotated by 18° in case of a non-completed carry.

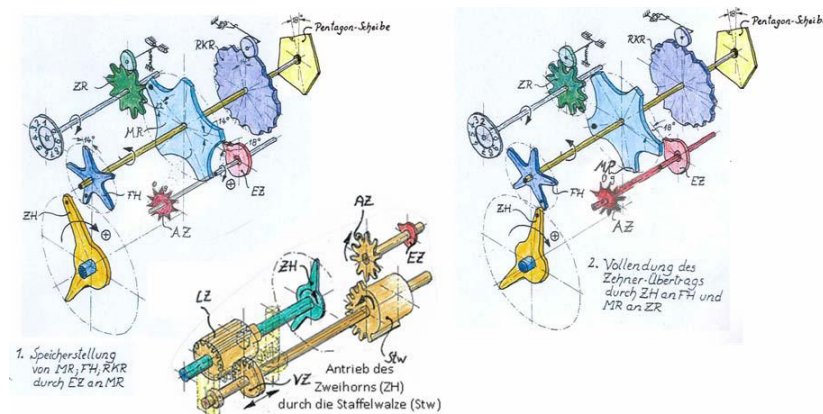


Figure 5: perspective of the decimal carry in Leibniz' four-species-calculator; 5a: first part of a decimal carry by the single horn (on the shaft of the recording wheel), rotating the five-bay-wheel (Muldenrad) by 18° ; 5b: twin horn (Zweihorn) between two neighbored stepped drums, rotated by the *Magna Rota* crank. All twin horns have the same spreading angle of 90° ; 5c: second part of decimal carry, as described in the above text.

For nearly 300 years it was claimed that Leibniz' calculator cannot operate correctly due to incomplete decimal carries, but only in the year 2004 when we set up and programmed the Pareto optimization of Leibniz' machine – especially for achieving complete decimal carries and minimizing imperfection sensitivities –, we found as a by-product, at first Klaus Badur, that complete decimal carries can be easily achieved by setting the multiplicand (or dividend) to zero in the input carriage and then rotate the *Magna Rota* crank – so to say idle – with 360° rotations, until all pentagon disks have returned to the original positions; thus all decimal carries are completed because this gear machine is a kinematic chain with one degree of freedom. And we also found the original records of Leibniz' co-workers with documented calculations, using the described slightly extended algorithms. This completely rehabilitates Leibniz' ingenious invention.

10. Leibniz' Replica with decaying Twin Horn Spreading Angles for Complete Decimal Carries by Nicolaus J. Lehmann

N. J. Lehmann, Technical University of Dresden, Germany, constructed and built in the 1980s some replicas of Leibniz' calculator with decreasing spreading angles of the twin horns of 32° to 35° between two places, beginning with the maximum possible angle, enabling 8 places for the digits of a number, figure 6. It is obvious that this yields sequential transfers of the digits from the input carriage to the calculating unit, and thus completes decimal carries. The design parameters in Lehmann's machine were not deduced from a mathematical optimization but from experimental trials and could not realize the complete decimal carries in the first exemplars.

11. Constructive and Mathematical Pareto Optimized Replica with decaying Twin Horn Spreading Angles by Erwin Stein and Franz Otto Kopp

In our Hannover Replica from 2004/2005 we performed Pareto optimizations of Leibniz' calculator with 3 goal functions and 8 to 12 design parameters for the decimal carries and the digit input, which will be

briefly described in the following section. It became obvious that the related algorithms can only converge on the basis of sequential transfer of digits into the calculating unit, i.e. on the basis of Lehmann’s replica.

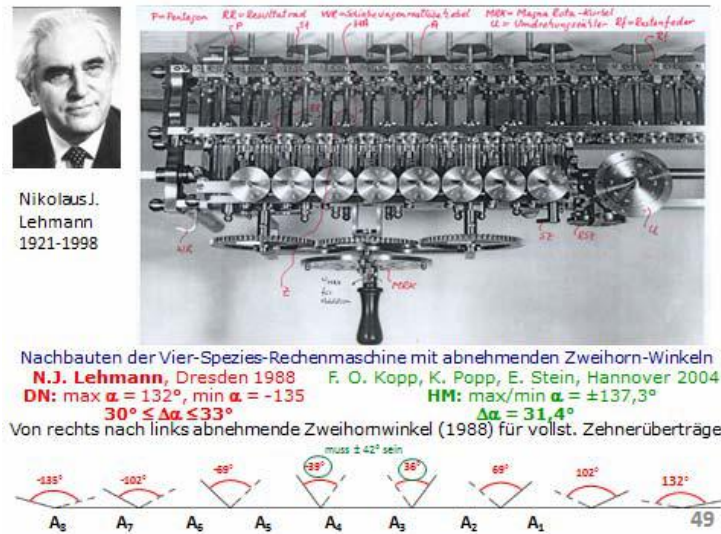


Figure 6: Replica by N. J. Lehmann with decaying twin horn-spreading angles for sequential transfer of digits for complete decimal carries.

The multi-objective-optimization of the Hannover replica was performed for the least-square-goal-function

$$f(x) = \underbrace{(\alpha_{GMR} - 18^\circ)^2}_{f_1} + \underbrace{(\alpha_{GZR} - 36^\circ)^2}_{f_2} + \underbrace{(\alpha_{ZHmax} - 90^\circ)^2}_{f_3} \rightarrow \min,$$

with the goal functions:

f1: for minimal deviation of the rotation of the five-bay-wheel from 18° in Leibniz’ machine,

f2: for minimal deviation of the rotation of the next left result wheel from 36°,

f3: for achieving the largest possible rightest spreading angle with the theoretical maximum of $2 \times 90^\circ = 180^\circ$,

for the 8 design parameter

$$x = [R_{MR}, R_{EZ}, R_{FH}, R_{ZH}, R_{ZR}, \alpha_{GMR}, \alpha_{GZR}, \alpha_{ZHmax}].$$

the 5 equality constraints are

$$h = [GNB1, GNB2, GNB3, GNB4, GNB5] = 0,$$

and the 6 inequality constraints are

$$g = [UNB1, UNB2, UNB3, UNB4, UNB5, UNB6] \leq 0.$$

The inequality constraints 1 to 3 and the equality constraint 1 and 2 for the rotation of the five-bay-wheel of the single horn and the non-contact sliding of the five-bay-wheel beneath the twin horn wheel in the second part of the decimal carry are:

$$\begin{aligned} \text{UNB1:} & R_{MR} \sin(\xi) - R_{EZ} \sin(18^\circ) \leq 0 \\ \text{UNB2:} & -\xi \leq 0 \\ \text{UNB3:} & \frac{(s/2) - R_{MR} \cos(\xi) - R_{EZ} \cos(18^\circ)}{\sqrt{(R_{MR}^2 - x_{EZ})^2 - (s/2)^2 \sin(18^\circ)^2}} \leq 0 \\ \text{GNB1:} & R_{EZ} - s/2 \cos(18^\circ) + \sqrt{(R_{MR}^2 - x_{EZ})^2 - (s/2)^2 \sin(18^\circ)^2} = 0 \\ \text{GNB2:} & \alpha_{GMR} - \gamma - \xi = 0 \end{aligned}$$

The 8 design parameters are depicted in figure 7.

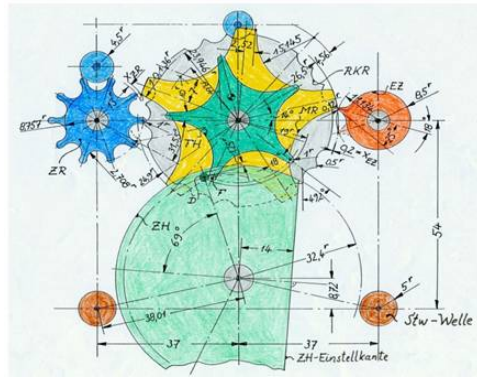


Figure 7: the 8 design parameters are the radii and angles of the gears for the decimal carries.

The penalized goal function $P(x, \epsilon)$ of shortest distance to the origin of the 8-dimensional function space is

$$P(x; \epsilon) = f(x) + \sum_{j=1}^5 \epsilon |h_j(x)| + \sum_{i=1}^6 \epsilon \max(0, g_i(x)) \quad ;$$

The numerical calculations are performed with genetic algorithms, followed by post-iterations with steepest descent method. The optimized solution vector with 8 design variables follows from multiple computational runs as, with all radii in millimeters:

$$\begin{aligned} x_{1opt} &= [R_1MR = 26.50; R_1EZ = 11.13; R_1FH = 19.00; R_1ZH = 31.45; R_1ZR = 13.00; \\ \alpha_{GMR} &= 13.84^\circ \text{ (instead of Leibniz' } 18^\circ); \alpha_{GZR} = 31.55^\circ \text{ (instead of Leibniz' } 21.5^\circ); \\ \max \alpha_{ZH} &= 68.66^\circ \text{ (max. twinhorn spreading angle } 2 \cdot 68.66 = 137.3^\circ); \end{aligned}$$

A further result was the optimized pitch angle between the stepped drum's teeth of $\varphi_{opt} = 21^\circ$, with the total angle of the stepped drum of $8 \cdot 21 = 168^\circ$, instead of $\varphi_{Leibniz} = 22.5^\circ$, with the total angle $8 \cdot 22.5 = 180^\circ$.

The Hannover replica, fig. 8, was constructed, optimized, and built in 2004/05 by K. Popp[†], E. Stein, and F.O. Kopp[†] in the workshop of the Institute of Mechanics, Universität Hannover. It has double distances of the stepped drums, compared against Leibniz' original machine, i.e. about twice the scale for demonstrating the machine exhibitions, and therefore only 6 instead of 8 input places, and 12 instead of 16 result places and 1 counting place at the input carriage; it is fully functional.

Complete Decimal Carries. In case of incomplete decimal carries, marked by rotated pentagon disks at related places, the optimization causes to rotate the *Magna Rota* crank by a further 87° , limited by a bolt, by which all decimal carries are completed. This means that the further **permissible rotation angle** – before executing a new addition or subtraction – is larger than the **required rotation angle** for completing the decimal carries. Exactly this is not fulfilled in Leibniz' machine; there is a missing angle of $\varphi_{admissible} - \varphi_{required} = -2,5^\circ$.

12. New Binary Four-Species Mechanical Calculator with the logics of Leibniz' decimal calculator, Designed, Constructed, and Built by E. Stein and F.O. Kopp[†] in 2007/08 at the Leibniz Universität Hannover

It is essentially possible to transfer the construction logic of mechanical calculators between different number bases b , e.g. from $b=10$ to $b=2$, or what was used in early electronic computers, $b=8$. In our implementation of this idea we were astonished about its simplicity, requiring only the change of 3 types of gear wheels, namely: (i) the step drums with only the digits 0 and 1, realized by bolts which are moved down for 1 and up for 0; (ii) the result wheels with 5 alternating 0s and 1s; and (iii) the initiation of the first part of binary carries by a five-horned wheel with alternating gaps and teeth (instead of the single horned wheel in the decimal machine), according to the rule $z = b \cdot r$ (number of teeth r is equal to the basis b times repetition r , with $z = 10$). It is remarkable for the ingenious design of Leibniz' decimal carries that the 4 gear wheels on one shaft remain unchanged for the transfer from $b=10$ to $b=2$. This binary machine was built with 7 input places, 12 result places, and 6 counting places, Fig. 8.

It should be remarked that this binary machine could only be constructed with decreasing spreading angles of the twin-horned wheels, according to the larger amount of places compared to the decimal system. This binary machine is fully functional.

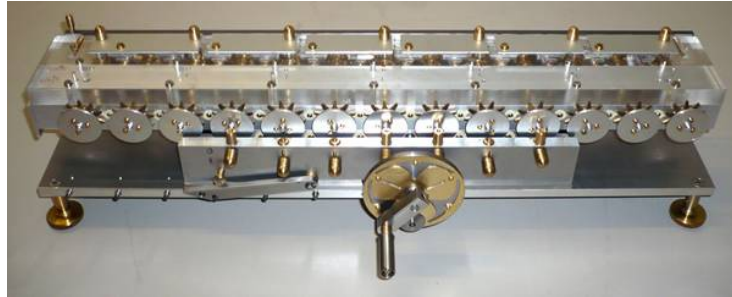


Figure 8: 7/12/6 placed binary four-species gear machine with only 3 changes with respect to the decimal machine.

13. Further Pieces in our Leibniz Exhibition and Closing Remarks

In addition to the presented calculators, we also constructed and built a fully functional binary two-species calculator with rolling steel bearings inside a sliding input carriage on a double skewed plane into the calculating unit with binary carry mechanisms, the *Machina dyadica*, as described by Leibniz in his unpublished manuscript *De progressionem dyadica* from 1679, where he introduced the binary number system and the 4 basic arithmetic operations.

Additionally, the second exemplar of the *Machina deciphatoria*, a cipher and deciphering machine, described by Leibniz in his minutes of his audience at the court of Kaiser Leopold I in Vienna, Austria, belongs to our exhibition. It is capable of $6 * 6! = 4,320$ ciphering combinations.

Leibniz was the first worldwide eminent German philosopher and universal scholar, with fundamental new contributions in all scientific branches of his time, especially pertaining to philosophy, legal and historical sciences, mathematics, mechanics, and moreover his ingenious technical inventions of decimal and binary calculators, technical improvements, and new transport systems *using the conjunction of wind and water* for silver ore mining in the Harz mountains. Last but not least, Leibniz invented the master plan for the improvement of the water works and the new 30 meter high fountain in the Herrenhäuser Gärten, for which we built about 20 functional models.

Finally, I would like to include some thought-provoking quotes from Leibniz:

- *All is connected with everything.*
- *Facts do not replace individual thought.*
- *He who seeks the truth should not count voices.*
- *Righteousness is the love of the wise.*
- *Theoria cum praxi combined with Bonum commune.*
- *Pars vitae quoties perditur hora perit (with every hour lost, you waste a part of your life)*

Figure 9 shows a bust of Leibniz portrayed as a Greek philosopher.

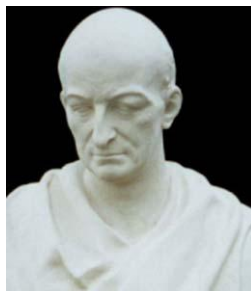


Figure 9: bust of Leibniz replica from the original bronzed plaster bust by Johann Gottfried Schmidt from 1788, based on the copper engraving of Leibniz by Martin Berningeroth, after the oil painting by Andreas Scheits

The world of Leibniz is the harmonic unification of matter, spirit and soul. Leibniz postulated the maxims *Unity of Science* with the program of a universal science, the unity of the real and the spiritual world, as a *Mathesis universalis*, the world of the monads in the best of all imaginable universes.

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Contributions in Infectious Diseases like the HIV/AIDS Epidemic

by Robert Murphy, Member EUAS

Short Biography

Professor of Medicine and Biomedical Engineering

My initial research experience began with the AIDS Clinical Trials Group (ACTG) of the National Institute for Allergy and Infectious Diseases/National Institutes for Health (NIH). My ACTG experience dates back to the founding of the network. I have been Principal Investigator (PI) of the Chicago Clinical Trials Unit for 18 years and have held many leadership positions in the network including memberships on many committees and working groups including: Adult Executive Committee, Data Management Committee (co-Chair), Hepatitis Transformative Study Group (TSG) and Hepatitis TSG Steering Committee. I have participated and led many clinical trials over the years and currently am co-Vice Chair of ACTG 5320 (V-HICS), a longitudinal study following patients treated for chronic hepatitis C with and without HIV.

I have extensive experience working in low- and middle-income countries (LMICs) and was the founding Nigeria Country Director of the Harvard Track 1.0 President's Emergency Plan for AIDS Relief (PEPFAR) program where we trained literally hundreds of clinicians and researchers who have subsequently treated over 150,000 HIV-infected Nigerians. My work with the NIH Fogarty International Center includes being PI of the AIDS International Training and Research Program (AITRP) in Nigeria and Mali, the Medical Education Partnership Initiative (MEPI) in Nigeria, three MEPI Junior Faculty Development training programs in Nigeria, an HIV and TB research training program in Mali, an HIV and Cancer research training program in Jos, Nigeria and a Biomedical Engineering Program development grant in Nigeria and South Africa. I've trained over 50 African scientists and have mentored more than 50 US Infectious Disease Fellows including 12 as primary mentor.

My mentoring experience includes very relevant training and oversight of programs in: Clinical Microbiology, Research Ethics, Biostatistics, Retrovirology, Mycobacteriology, Clinical Investigation, Pharmacology, Pediatric HIV, and Faculty Enrichment (grant writing, manuscript writing, research methodology).

Positions and Employment

1986 - 1990	<i>Assistant Professor of Medicine, Northwestern University, Chicago, IL</i>
1990 - 1999	<i>Associate Professor of Medicine, Northwestern University, Chicago, IL</i>
1999 -	<i>Conseil d'Administration, Objectif Recherche Vaccin SIDA (Paris), Paris</i>
1999 -	<i>Professor of Medicine, Northwestern University, Chicago, IL</i>
2004 -	<i>Visiting Professor of Immunology and Infectious Diseases, Harvard School of Public Health, Boston, MA</i>
2007 - 2008	<i>Professeur Associé, Université Pierre et Marie Curie, Paris</i>
2009 -	<i>Director, Center for Global Health, Northwestern University, Chicago, IL</i>
2013 -	<i>Professor of Medicine and Biomedical Engineering, Northwestern University, Chicago and Evanston, IL</i>

Other Experience and Professional Memberships

2002 -	<i>Co-Chair, Data Management Committee, ACTG/NIAID/NIH</i>
2004 -	<i>Member, Adult Executive Committee, ACTG/NIAID/NIH</i>
2005 - 2010	<i>Member, Merit Review Subcommittee of Infectious Diseases, Veterans Administration</i>
2008 -	<i>Senior Editor Virology, Journal of Antimicrobial Chemotherapy</i>

- 2011 - *Member, Hepatitis Transformative Study Group and Steering Committee, ACTG/NIAID/NIH*
- 2011 - 2015 *Member, AIDS Immunology and Pathogenesis Study Section, Center for Scientific Review/NIH*
- 2012 - *Director, Extramural Programs in HIV and Tuberculosis, SEREFO Laboratories, University of Bamako (USTTB) Mali*
- 2013 - *Faculty Director, Masters of Science in Global Health, Northwestern University*
- 2016 - *Member, International and Cooperative Projects I Study Section, Center for Scientific Review/NIH*

Honors

- 1975 *A.B. magna cum laude, Biology, Boston University*
- 1994 *AIDS Physician of the Year Chicago, Chicago Magazine*
- 2001 *John P. Phair Professor of Infectious Diseases, Northwestern University*
- 2005 *Founder's Award, Chicago House*
- 2006 *Fellow, Institute of Medicine of Chicago*
- 2007 *Global Health Humanitarian Award, Chicago Institute of Medicine*
- 2011 *Paul Harris Fellow, Rotary International, Polio Eradication Project*
- 2013 *Honorary Doctor of Humanities, Southern Illinois University*
- 2017 *Prix du Partenariat, Université des Sciences, des Techniques et des Technologies de Bamako*

Contribution to Science

1. I began my fellowship in infectious diseases just as the HIV/AIDS epidemic was taking off in Chicago. At one time early on in the epidemic, I was treating approximately one third of the patients with AIDS in Illinois and admitted more patients to Northwestern Memorial Hospital than any other staff physician. This situation was very intense and motivated me to discover optimal treatments for HIV infection starting with zidovudine monotherapy. This evolved over the years to include my studying essentially every antiretroviral drug that is marketed today and many of the immunotherapeutics. I was an early investigator in the NIH AIDS Clinical Trials Group where I led many clinical study teams and held leadership positions including membership on the Executive Committee, Scientific Agenda Steering Committee and Data Management which I still chair today among others. I participated in many international networks as well, including the French therapeutic vaccine group, Objectif VACCIN SIDA (ORVACS). My research is now focused primarily on early drug and therapeutic vaccine development and on cure strategies.
 - a. Wilkinson J, Ewart G, Luscombe C, McBride K, Ratanasuwan W, Miller M, **Murphy RL**. A Phase 1b/2a study of the safety, pharmacokinetics and antiviral activity of BIT225 in patients with HIV-1 infection. *J Antimicrob Chemother.* 2016 Mar;71(3):731-8. PubMed PMID: [26620101](https://pubmed.ncbi.nlm.nih.gov/26620101/).
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- d. **Murphy RL**, Autran B, Katlama C, Brucker G, Debre P, Calvez V, Clotet B, Clumeck N, Costagliola D, Deeks SG, Dorrell L, Gatell J, Haase A, Klein M, Lazzarin A, McMichael AJ, Papagno L, Schacker TW, Wain-Hobson S, Walker BD, Youle M. A step ahead on the HIV collaboratory. *Science*. 2009 Jun 5;324(5932):1264-5. PubMed PMID: [19498149](#).
2. I have a strong interest in studying co-infection with hepatitis C (HCV) and hepatitis B (HBV). These dual viral infections in the face of HIV are devastating with very rapid progression to end stage liver disease and hepatocellular cancer. Most of the work I have done in co-infection has been in Nigeria. I led the group describing the extent of co-infection status in Nigeria and was one of the first to use the Fibrosan[®] (transient elastography), to study liver stiffness or fibrosis in Africa. This interest has led to my junior colleague, Claudia Hawkins, being awarded a K23 award to study HIV/HBV co-infection in Tanzania. Within the AIDS Clinical Trials Group, I am a member of the Hepatitis Transformative Science Group and its Steering Committee and participate in its Hepatitis B Cure Working Group.
- a. Idoko J, Meloni S, Muazu M, Nimzing L, Badung B, Hawkins C, Sankalé JL, Ekong E, **Murphy R**, Kanki P, Thio CL. Impact of hepatitis B virus infection on human immunodeficiency virus response to antiretroviral therapy in Nigeria. *Clin Infect Dis*. 2009 Oct 15;49(8):1268-73. PubMed PMID: [19772386](#); PubMed Central PMCID: [PMC2753765](#).
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- c. Agbaji O, Thio CL, Meloni S, Graham C, Muazu M, Nimzing L, Idoko J, Sankalé JL, Ekong E, **Murphy R**, Kanki P, Hawkins C. Impact of hepatitis C virus on HIV response to antiretroviral therapy in Nigeria. *J Acquir Immune Defic Syndr*. 2013 Feb 1;62(2):204-7. PubMed PMID: [23196830](#); PubMed Central PMCID: [PMC3548937](#).
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- e. Grant J, Agbaji O, Kramvis A, Yousif M, Auwal M, Penugonda S, Ugoagwu P, **Murphy R**, Hawkins C. Hepatitis B virus sequencing and liver fibrosis evaluation in HIV/HBV co-infected Nigerians. *Top Med Int Health*. 2017 [Epub ahead of print]

3. Over the past 15 years, I have focused my effort on research infrastructure development in Africa, primarily Nigeria and Mali. I was the founding Nigeria Country Director for the Harvard President's Emergency Plan for AIDS Relief (PEPFAR). The development of this vital infrastructure led to subsequent awards from Fogarty (Medical Education Partnership Initiative [MEPI], AIDS International Training and Research Program [AITRP]), research training programs in Mali and Nigeria and Frameworks. The Frameworks grant is notable for the collaboration with my colleagues at Northwestern's McCormick School of Engineering and Kellogg School of Management. We have started to develop critically needed diagnostic products and biomedical engineering programs at the Universities of Ibadan and Lagos in Nigeria. 10 years ago, I began working with Malian investigators on developing their HIV and TB research programs. I oversaw training for 18 junior scientists in molecular virology, microbiology, clinical investigation and pharmacology. In 2012, I became the Director for Extramural HIV and TB Research, a position I hold today.
- a. Musa J, Nankat J, Achenbach CJ, Shambe IH, Taiwo BO, Mandong B, Daru PH, **Murphy RL**, Sagay AS. Cervical cancer survival in a resource-limited setting-North Central Nigeria. *Infect Agent Cancer*. 2016;11:15. PubMed PMID: [27014366](#); PubMed Central PMCID: [PMC4806480](#).
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Recent Improvements in Nuclear Engineering

by Piero Ravetto, Member EUAS

Short Biography

Politecnico di Torino, Dipartimento Energia

- *Researcher at Politecnico di Torino from 1.11.1974 till 31.10.1978; in the period 1.1.1975 - 31.3.1976 on leave at Dragon Project, General Physics and Dynamics Group, Atomic Energy Establishment, Winfrith, United Kingdom;*
- *Associate professor of Nuclear Reactor Physics at Politecnico di Torino from 1.11.1978 till 28.2.2000;*
- *Full Professor of Nuclear Reactor Physics at Politecnico di Torino since 1.3.2000; Head of the Energy and Nuclear Engineering Program at Politecnico di Torino, October 2003-September 2012.*

Scientific Board and Professional Society Membership

- *Fellow of the American Nuclear Society;*
- *Member of the Scientific Board of the Frédéric Joliot – Otto Hahn School in Reactor Physics;*
- *Member of the Organizing Committee for the International Conference on Transport Theory, from the 15-th to the 24-th editions;*
- *Member of the organizing committees of several international conferences and topical meetings sponsored by the American Nuclear Society; organizer of many special sessions for the reactor physics and mathematics and computation divisions;*
- *Member of the Executive Committee of the Mathematics and Computation Division of the American Nuclear Society (since 2000); secretary of the Division for the year 2002/2003; member of the honor and awards committee;*
- *Member of the scientific evaluation committee for CEA (France) activities in nuclear reactor physics, 2003;*
- *Member of the scientific evaluation committee for IRSN (France) activities in nuclear reactor physics, 2012;*
- *Member of the Independent Review Committee for the project An innovative hybrid deterministic/Monte Carlo radiation transport method for modelling radiation sensor systems, DOE, Battelle Pacific Northwest National Laboratory – Atlanta, April 2011;*
- *Expert reviewer on behalf of DOE-NE's Consolidated Innovative Nuclear Research Program, 2013-2015;*
- *Member of several evaluation committees for university professorship positions (Italy, USA, Taiwan, The Netherlands).*

Most significant teaching and seminar activity:

- *Three Dimensional Transport Methods for Core Calculations: Basic Theory - Frédéric Joliot Summer School in Reactor Physics – Centre d'Etudes Nucléaires, CEA, Cadarache (France), 1995;*
- *Dynamics of Subcritical Systems, Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety, Abdus Salam International Centre for Theoretical Physics, Trieste (Italy), 2000;*
- *Lectures on reactor physics at the Summer School on Challenges for energy supply and environmentally sound development, Beijing/Harbin, July 2006, July 2007;*
- *Nuclear Reactor Dynamics, Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety, Abdus Salam International Centre for Theoretical Physics, Trieste (Italy), 2002-2009;*
- *Accelerator-Driven Systems Dynamics, Workshop on Accelerator-Driven Systems, organized by IAEA, 2003, 2005 and 2007;*

- *Introduction to neutronics and core physics: current code capabilities, Frédéric Joliot and Otto Hahn Summer School on Nuclear Reactor Physics, Fuels and Systems on High-Fidelity Modelling for Nuclear Reactors: Challenges and Prospects, Karlsruhe – August 2011;*
- *Modern challenges in transport theory, Wilhelm und Else Heraeus Seminar on Innovative Nuclear Power in a Closed Fuel Cycle Scenario, Bad Honnef – December 2011;*
- *Neutron transport theory and numerical methods for reactor physics applications, KIT, Karlsruhe – July 2012;*
- *Nuclear reactor theory – at the IAEA training course to support nuclear power programme for APEC Countries, Malaysia Nuclear Agency, Kuala Lumpur – August 2013;*
- *Many seminars at Italian, European and American Universities and Research Centres.*

S. Dulla, M. Nervo, P. Ravetto, A method for the continuous monitoring of the reactivity in subcritical source-driven systems, *Annals of Nuclear Energy*, 87, 1-11 (2015).

In the present work the problem of the on-line monitoring of the reactivity in a source-free nuclear reactor is considered. The method is based on the classic point kinetic model of reactor physics. A relationship between the instantaneous value of the system stable period and the values of the neutron flux amplitude (or the power), of its derivative and of the integral convolution term determining the instantaneous value of the effective delayed neutron concentration is derived. The reactivity can then be evaluated through the application of the inhour equation, assuming the effective delayed neutron fraction and prompt generation time are known from independent measurements. Since the power related quantities can be assumed to be experimental observables at each instant, the reactivity can be easily reconstructed. The method is tested at first through the interpretation of power histories simulated by the solution of the point kinetic equations; the effect of the time interval between power detections on the accuracy is studied, proving the excellent performance of the procedure. The work includes also a study on the sensitivity of the reactivity forecast to the uncertainty on the values of the effective delayed neutron fraction and prompt generation time. The spatial effects are investigated by applying the method to the interpretation of flux evolution histories generated by a numerical code solving the space-time dependent neutron kinetic equations in the diffusion model. Also in this case the method proves to be quite effective in providing good estimates of the system reactivity, except at very short times after the introduction of a perturbation inducing a spatial transient. At last, the effect of the experimental noise is investigated, proving that the consequences in the accuracy of the reactivity prediction can be mitigated by using an adequate differentiation algorithm.

A. Barbarino, S. Dulla, E.H. Mund, P. Ravetto, The spectral element method for neutron transport in AN approximation. Part I, *Annals of Nuclear Energy*, 53, 372-380 (2013).

Spectral elements methods provide very accurate solutions of elliptic problems. In this paper we apply the method to the AN (i.e. SP2N-1) approximation of neutron transport. Numerical results for classical benchmark cases highlight its performance in comparison with finite element computations, in terms of accuracy per degree of freedom and convergence rate. All calculations presented in this paper refer to two-dimensional problems. The method can easily be extended to three-dimensional cases. The results illustrate promising features of the method for more complex transport problems.

A. Barbarino, S. Dulla, E. Mund, P. Ravetto, The spectral element method for neutron transport in AN approximation. Part II, *Annals of Nuclear Energy*, 86, 108-115 (2015).

This paper is the second part of an investigation on the use of the spectral element method (SEM) to solve neutron transport problems in the AN approximation. Part I of the study contained a description of the SEM variational approach of the AN equations applied to classical assembly benchmark problems. Part II deals with the SEM solution of these equations in reactor cells. To cope with the cell geometry we apply a mapping technique from curved to square domains based on transfinite interpolation. Benchmark exercises – based on the method of characteristics – on the scale of fuel cells give a further confirmation of the computation advantages of the SEM-AN approach in comparison with classical low-order computational techniques.

S. Dulla, M. Nervo, P. Ravetto, A method for the continuous monitoring of the reactivity in subcritical source-driven systems, *Annals of Nuclear Energy*, 87, 1-11 (2015).

The reactivity monitoring in subcritical accelerator-driven systems is a key aspect for the development of this technology. In this work, an inverse method for the determination of the system reactivity from the analysis of flux and power signals, based on the point kinetic approach, is applied to source-driven systems.

The features of the algorithm specific to the application to subcritical assemblies are identified, and the sensitivity to the integral parameters characterizing the system is discussed. The technique is applied to different transient situations, simulated by neutronic codes adopting point kinetics and multigroup diffusion, and its accuracy in the presence of localized spatial and spectral phenomena is assessed. Different approaches for the reduction of the uncertainties introduced by the experimental noise are proposed and compared.

D. Caron, S. Dulla, P. Ravetto, Adaptive time step selection in the quasi-static methods of nuclear reactor dynamics, *Annals of Nuclear Energy*, 105, 266-281 (2017).

Of the methods available by which to integrate the neutron and delayed neutron precursor balance equations in time, at present the quasi-static methods are among the most practical and favourable. However, the correct application of the quasi-static method requires the use of appropriately determined time steps, for both the reasons of accuracy and efficiency. This work presents a methodology for the adaptive selection of the time steps employed by the quasi-static method, thereby allowing the quasi-static approach to be applied in an efficient manner while maintaining a prescribed level of accuracy. The method is applied to and studied using some numeric test problems.

S. Dulla, S.S. Hoh, G. Marana, M. Nervo, P. Ravetto, C.H. Pyeon, Analysis of KUCA measurements by the reactivity monitoring MAPTA method, *Annals of Nuclear Energy*, 101, 397-407 (2017).

A recently developed method for the continuous reactivity monitoring in nuclear reactors and in subcritical source-driven systems is applied for the interpretation of flux measurements carried out in the KUCA facility. The scope of the work is to validate the method using real experimental data. The method is based on general mathematical properties of the differential equations constituting the point kinetic model. Several pulsed experiments performed in different system configurations and using different source target materials are analysed. The results are compared with the classic area ratio method. A good agreement is obtained when the space-energy transient following the source shut-down dies out and when the system sets on a point-like evolution. The results prove the suitability of the proposed method for application to the reactivity monitoring of source-driven systems.

S. Dulla, A.K. Prinja, P. Ravetto, Random effects on reactivity in molten salt reactors, *Annals of Nuclear Energy*, 64, 353-364 (2014).

The problem of the effect of fissile lumps spatially appearing in a random fashion inside a fluid fuel reactor is addressed. The effect on static reactivity is evaluated by means of first-order perturbation theory. The analysis is carried out in diffusion theory with the presence of delayed neutron emissions, taking into account the fuel motion that introduces a distortion of the space distribution of the delayed neutron precursors. The method is applied to a one-dimensional configuration to investigate the general features of the random process. Afterwards, a more realistic two-dimensional cylindrical geometry is considered. The estimation of the mean value and standard deviation of the reactivity inserted is performed by Monte Carlo simulations and a deterministic quadrature approach, to compare the methods in terms of computational effort and accuracy of the results. The reconstruction of the probability density function of the reactivity is also performed by polynomial chaos expansion. The results presented show that random reactivity effects constitute an important issue in the assessment of these innovative molten salt systems.

S. Dulla, E.H. Mund, P. Ravetto, The Quasi-Static Method Revisited, *Progress in Nuclear Energy*, 50 (8) 908-920 (2008).

The quasi-static method is a standard tool for the space-time solution of neutron transport problems in multiplying media. Its basic principle lies in a factorization of the angular flux into the product of two functions, 'amplitude' and 'shape', where the amplitude depends only on time (and contains the major part of the time-dependence) while the shape function depends on all variables, time included. The shape equation is solved on a long time-scale, while the amplitude is determined on a short time-scale. The factorization is made unique by proper normalization conditions for the shape function. Most implementations replace the basic equation (transport or diffusion) by the set of coupled amplitude and shape equations derived from the factorization, the so-called 'Improved Quasi-static Method' (IQM). In this paper we describe an alternate approach already known for some time we have called 'Predictor-Corrector Quasi-static Method' (PCQM). We discuss its efficiency for both solid- and liquid-fuel systems dynamics.

Research about Time Effects in Rock Mechanics

by **Nicolaie Cristescu, Member EUAS**



Short Biography

Corresponding member (9 March 1991) and member (11 December 1992) of the Romanian Academy. Member of the EU Academy of Sciences (2015). He attended the Faculty of Mathematics and Physics of the University of Bucharest; he obtained his PhD in mathematics and physics in 1955; he obtained his PhD docent in 1967. He was an assistant at the Institute of Geology and Mining Technique (1950-1951), then assistant (1951-1955), lecturer (1955-1957), professor associate (1957-1966) and professor (1966); Head of Department (1982-1990) at the University of Bucharest, whose rector was (1990-1992); "Visiting professor" at The Johns Hopkins University, Baltimore (1968-1969), consulting professor at Drexel Institute of Technology in Philadelphia (1969), Professor (1970) and "The Graduate Research Professor" (1971-1976, 1992-2009) at the University of Florida, Gainesville. His research addresses various fields: the theory of plasticity and viscoplasticity, wave propagation, rock mechanics, mechanics of composite materials, theory of metalworking processes, mechanics of granular materials. From 1953 he worked in the theory of plasticity, hitherto unexplored in Romania and which proved of great importance in many areas of technology (metalworking, earth and rock mechanics, plastics, powders etc.). He was concerned about the mechanics of "composite" bodies and at the request of metallurgical enterprises and the Metallurgical Research Institute, developed mathematical models to describe various metalworking processes. His research of elastic-plastic materials processes and for the establishing of the constitutive equations for these materials have diversified over time by a mechanical approach to composite materials and suggesting a mechanism of sequential delamination; he gave a new theory of slow deterioration of rocks by dilatant and a correlation between mechanical effects and acoustic emission. Following a contract with a group of geomechanics researchers, he made a number of applications in mining: the calculation of vertical and horizontal holes in mining, taking into account the deterioration in time. The results of his research were published in more than 200 papers, published in our country and abroad, under own signature or in collaboration with other specialists. Among the books published we mention: Dynamic Problems in Plasticity Theory (1958); Mechanical of Fibers Elongation (1964, published in Chinese); Dynamic Plasticity (1970, published also in Japanese); Introduction to Rate-dependent Plasticity (a Dynamic Approach) (1971); Viscoplasticity (1982 et al.); Mechanics of Composite Materials (1983); Rock Mechanics (1984); The Theory of Plasticity in Metalworking Applications (1985 et al.); Rock and Soil Rheology (1988, et al.); Rock Rheology (1989); Rock Mechanics-Rheological Aspects

(1989); *Visco-Plastic Behavior of Geomaterials* (1994 et al.); *Time Effects in Rock Mechanics* (1997 et al.); *Basic and Applied Salt Mechanics* (2002, et al.); *Mechanics of Elastic Composites* (2003 et al.); *Dynamic Plasticity* (2007). Editor-founder of the journal "International Journal of Plasticity", a member of the editorial committee of the magazines "International Journal of Mechanical Sciences", "International Journal of Impact Engineering", "Mechanics Research Communications", "Mechanics of Cohesive-Frictional Materials", "Revista Italiana di Geotecnica". Member of the European Mechanical Committee, founding member of the International Society for Interaction of Mechanics and Mathematics, member of the American Society of Mechanical Engineers, member of the Society Sigma XI, of the French Group of Rheology, member of the Academy Europaea (1997).

The use of underground space is increasing in our time. The reason is the increase of world population, and due to our increasing demand. Storage for liquids, gases and various demands of underground storage. Also, many large underground spaces like travel tunnels, caverns for power stations and storage facilities are now excavated. Mines are going deeper as are wellbores. In addition, materials more difficult to handle, and to be described by mathematical models, are involved. Due to this, the design and construction is becoming increasingly sophisticated. The short term and long term deformation and stability has to be predicted with increasing accuracy and the time scales involved are becoming much longer. Therefore, a purely empirical approach is not reliable enough. The appropriate theoretical background especially for the constitutive equations describing the time dependent reactions of the rocks affected by the excavation, is to be involved. This also has a considerable influence on the experimental requirements, since more accurate experimental devices and methods are needed.

Rock mechanics is related to structural geology, soil mechanics, materials sciences, civil, mining and petroleum engineering, seismology and geophysics.

The content of the research concentrates on elasticity, creep, dilatancy, creep failure, short term failure, viscoplasticity and related effects, its measurement and the description by appropriate constitutive equations.

The constitutive equation is:

$$\dot{\epsilon} = \frac{\dot{\sigma}}{2G} + \left(\frac{1}{3K} - \frac{1}{2G}\right)\dot{\sigma} + k_T \left(1 - \frac{W(\epsilon)}{H(\sigma)}\right) \frac{\partial F}{\partial \sigma} + k_s \frac{\partial S}{\partial \sigma}$$

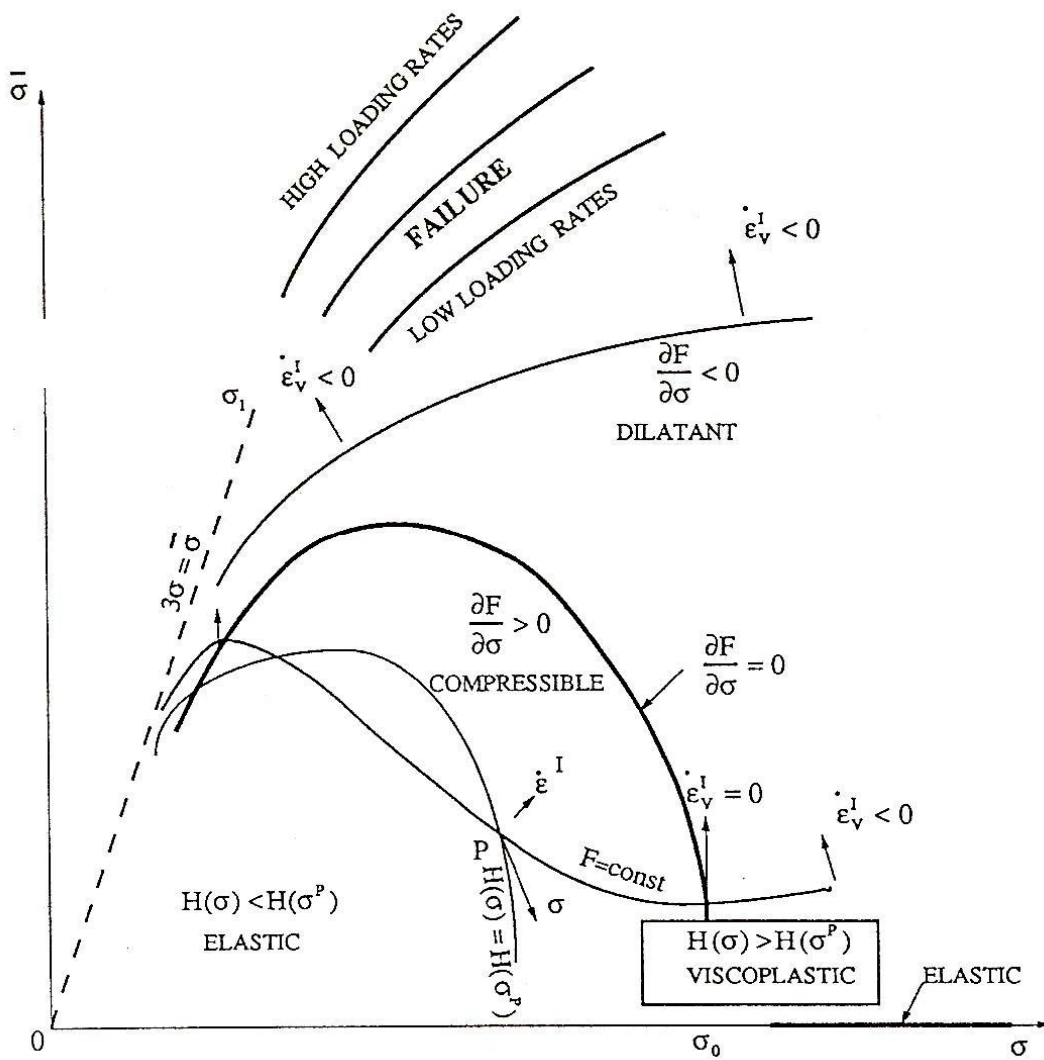
Where

$$\frac{\partial F}{\partial \sigma} \cdot \mathbf{1} > 0 \quad \text{or} \quad \frac{\partial F}{\partial \sigma} > 0 \quad \text{compressibility}$$

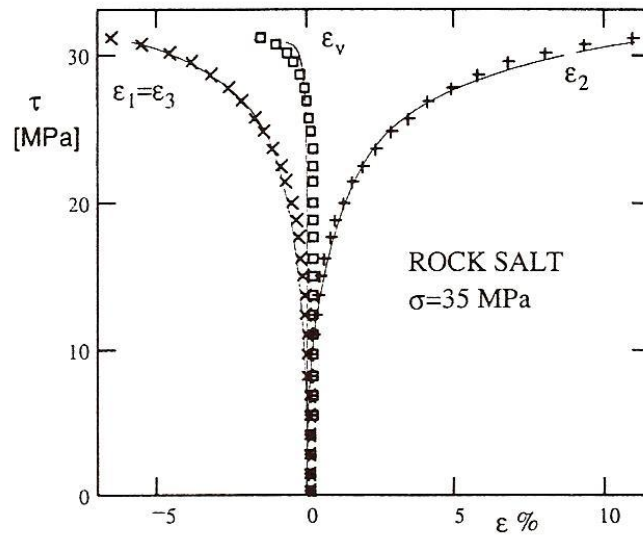
$$\frac{\partial F}{\partial \sigma} \cdot \mathbf{1} = 0 \quad \text{or} \quad \frac{\partial F}{\partial \sigma} = 0 \quad \text{compressibility/dilatancy boundary}$$

$$\frac{\partial F}{\partial \sigma} \cdot \mathbf{1} < 0 \quad \text{or} \quad \frac{\partial F}{\partial \sigma} < 0 \quad \text{dilatancy}$$

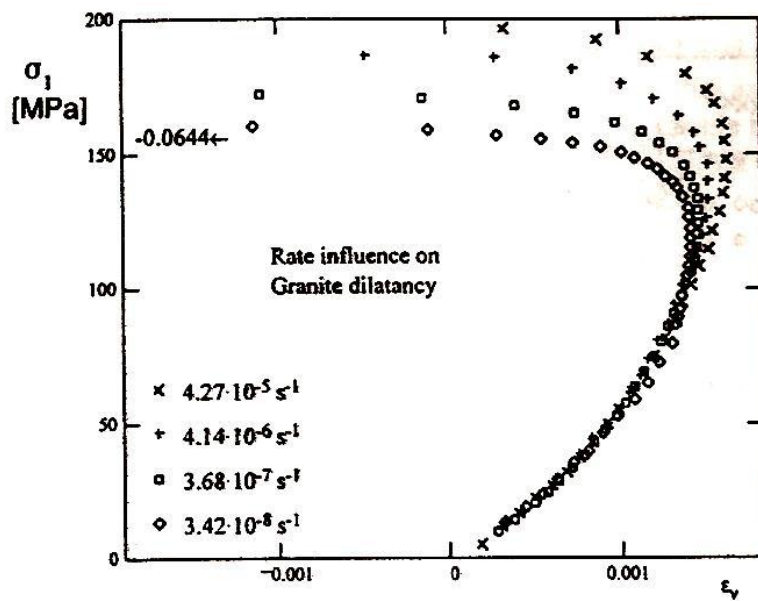
All the explanations are on the figure:



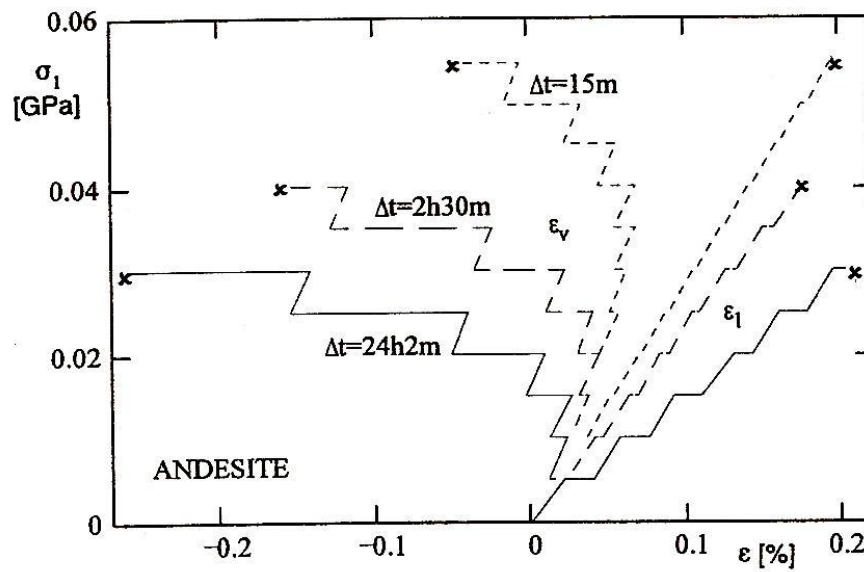
The behavior on the figure below is showing what a constitutive equation is:



The figure below is showing the strain-rate influence on granite:

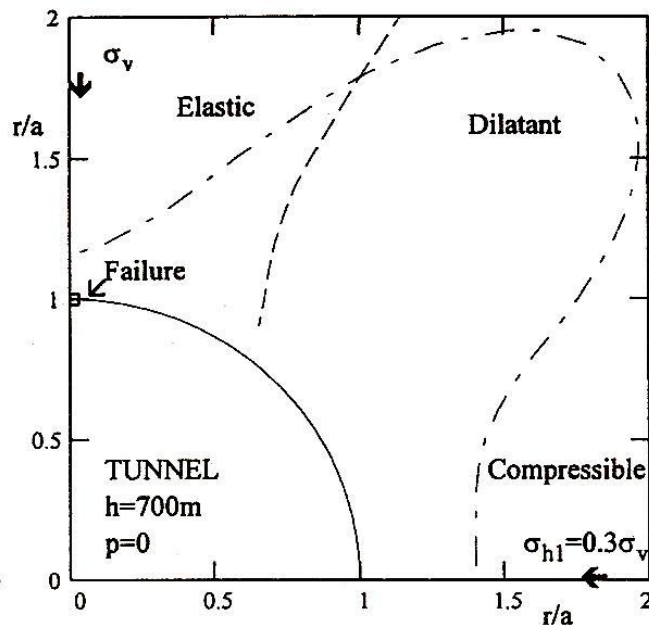


The incremental creep tests for andesite is shown in the figure below:



The stress is kept constant for the time interval shown.

The domains of dilatancy, compressibility, and failure around a tunnel was studied. In the next figure is shown one such case:



The tunnel failure can be described by scientific approach.

Novel Semi-Conductor Nanostructures

by Dieter H. Bimberg, Member EUAS



Short Biography

Dieter H. Bimberg, received the Diploma in physics and the Ph.D. degree from Goethe University, Frankfurt, in 1968 and 1971, respectively. From 1972 to 1979 he held a Principal Scientist position at the Max Planck-Institute for Solid State Research in Grenoble/France and Stuttgart. In 1979 he was appointed as Professor of Electrical Engineering, Technical University of Aachen.

In 1981 he was appointed to the Chair of Applied Solid State Physics at Technical University of Berlin. He was elected in 1990 Executive Director of the Solid State Physics Institute at TU Berlin, a position he held until 2011. In 2004 he founded the Center of Nanophotonics at TU Berlin. From 2006 to 2011 he was the chairman of the board of the German Federal Government Centers of Excellence in Nanotechnologies.

His honors include the Russian State Prize in Science and Technology 2001, his election to the German Academy of Sciences Leopoldina in 2004, to the Russian Academy of Sciences in 2011, to the US National Academy of Engineering in 2014, and to the US National Academy of Inventors 2016, as Fellow of the American Physical Society and IEEE in 2004 and 2010, respectively, the Max-Born-Award and Medal 2006, awarded jointly by IoP and DPG, the William Streifer Award of the Photonics Society of IEEE in 2010, the UNESCO Nanoscience Medal 2012, and the Heinrich-Welker-Award and medal in 2015. The University of Lancaster bestowed in 2015 a D.Sc.h.c. to him. In 2017 the Chinese Academy of Sciences appointed him as Einstein Professor.

He has authored more than 1500 papers, 30 patents, and 6 books resulting in more than 53,000 citations worldwide and a Hirsch factor of 101 (@ google scholar).

His research interests include the growth and physics of nanostructures and nanophotonic devices, ultrahigh speed and energy efficient photonic devices for future datacom systems, single/entangled photon emitters for quantum cryptography and ultimate nanomemories based on quantum dots.

Scientific Achievements

Dieter Bimberg is one of the world's leading semiconductor physicists. He has made major, even spectacular, breakthroughs in research on semiconductor nanostructures, in particular quantum dots. His work has originally focused on experimental and theoretical studies of nanostructure growth, with concomitant computer-based numerical modelling, as well as on their electronic/excitonic and optical properties. These studies, based in part on novel modelling and measuring techniques, such as cathodoluminescence and calorimetric absorption spectroscopy have opened up a new area of physics. He discovered very unusual physical properties like size dependent and negative bi-exciton binding energies or sign inversion of excitonic fine structure splitting. His subsequent development of nanostructures as gain or carrier storage materials with properties depending on size and

shape of the quantum dots, have paved the way for photonic and memory devices with revolutionary properties. Single and entangled q-bit emitters for quantum communication, nano-flash memories for “beyond Moore computers”, dual direction semiconductor optical amplifiers and energy-efficient surface emitting lasers for ultrahigh speed optical interconnects in data centres exemplify the wide field of devices he pioneered. His work is characterized by a visionary scientific approach in which experiment, theory based on numerical modelling and device development have been pursued in strategically decisive areas combining materials science, nanophysics, measurement technology, nano-photonic and -electronic devices and quantum communication.

In materials science he and his co-workers have studied the fundamentals of self-organization of strained layers at surfaces of semiconductors, both theoretically and experimentally (using molecular beam epitaxy and metal-organic chemical vapour-phase deposition, MBE and MOCVD, respectively), in order to understand and then control the growth of quantum dots. He discovered that it is the surface strain tensor, which enforces self-organization at the surfaces of cubic or wurtzite III-V compounds. This in turn has enabled the fundamental observation of self-ordering at the surfaces of such materials to be explained. In basic nanophysics Bimberg has modelled the electronic properties of quantum dots and the electron-phonon interaction, using effective mass theory followed by complex 8-band $k\cdot p$ -theory. This pioneering work has initiated follow-up activities worldwide. His discovery and experimental confirmation of the constant two-fold degeneracy of any energy level in quantum dots has paved the way for applications of single quantum dots in quantum communication. His extension of the theoretical work to include many-body interactions (exchange and correlation) enabled for the first time predictions to be made as to the size and shape dependence of excitonic fine structure splitting and negative or zero bi-excitonic binding energies in numerical agreement with his experimental observations. His development of cathodoluminescence as a laterally resolved optical technique with high temporal resolution led to the first observation of the delta-function character of single QD emission lines, the excitonic fine-structure splitting and its dot size dependence. His ultrasensitive calorimetric absorption spectroscopy allows a quantitative assessment of sources of non-radiative recombination. The first injection laser based on Stranski-Krastanow quantum dots was introduced by Bimberg and group in the beginning of the nineties, originally at 77 K and shortly afterwards at room temperature. Systematic successive research and development have led to novel ultrahigh speed nanophotonic devices, like mode-locked or directly modulated lasers for high speed/bit rate optical interconnects, metro and access communication systems for an energy efficient internet. Finally he has suggested the nanoflash memory, combining the best of flash and DRAM and demonstrated its feasibility with 4 days storage time at present.

In summary, Dieter Bimberg, drawing on outstanding experimental skills and deep theoretical insight, has over the years initiated new and exciting areas of semiconductor physics and device research that have led to applications presenting brake-throughs. He is acknowledged as a world-leader of extraordinary achievements in these fields. He is Professor of Applied Physics at the Institute of Solid State Physics and Founding Director of the Centre for Nanophotonics at the Technical University of Berlin. More than 1500 research publications, 53000+ citations, and a Hirsch factor of 101 (Google Scholar) demonstrate the enormous influence of his work and its impact on science.

Contributions to Society based on the above-mentioned Achievements

Dieter Bimberg has developed novel semi-conductor nanostructures, in particular quantum dots and their arrays and stacks, as gain or memory materials with size- and shape-dependent characteristics. Very early in his research he realized that thus the electronic or optical properties of such nanomaterials, as the emission wavelength of a laser, can be varied across large parameter ranges without changing the composition of the material or the use of rare materials. Semiconductor lasers could cover now wavelength windows in e.g. the infrared spectrum, which could not be covered before his discovery. Gain recovery time in nanolasers emitting pulses on the ps- and fs-time scale was observed to be orders of magnitude faster than in classical semiconductor lasers, thus allowing much larger bit rates in data communication, reducing the need of multiplexing devices and saving enormous amounts of energy. He called this new way of influencing material properties “geometrical architecture“.

His discovery of the very unusual physical properties of nanostructures has enabled him to build novel photonic and electronic devices. Soon he realized the enormous contributions he could make towards solving pressing problems of our society. Most important to him appeared the challenges of our energy-hungry and security-conscious information society. Rapidly expanding internet traffic will use up almost all the electrical energy produced around 2022, if now radical reduction of energy use of interconnects and computers via “green” photonic or memory devices is achieved. Examples of novel devices he developed are energy efficient nano-flash memories for “beyond Moore integrated circuits” based on the capture of just a few carriers in type II quantum dots, energy-efficient surface emitting lasers for ultrahigh speed optical interconnects in data centres or broad band semiconductor optical amplifiers for energy efficient ultrafast amplification and signal processing in local and metropolitan area networks, to mention a few. Electrically driven high-speed single and entangled q-bit emitters developed by him are of equal importance for practical room temperature user-friendly quantum communication and cryptography.

The first electrically driven quantum dot lasers were introduced by Bimberg and his group in the beginning of the 1990’s. With 160 GHz pulses, a few hundred fs pulse-width, ultra-low jitter of a few tens of femtosecond and low chirp observed from his mode-locked quantum dot lasers at the communication wavelength of 1310 nm he is still the leader in this field. These innovations provide the enabling technology for upstream communication in local area networks.

He presented the first surface emitting lasers with oxide aperture operating at the ground state of quantum dots and a sensational low-threshold current of 68 μA in 1997. He developed his own post-growth processing technologies, based on novel multiple oxide apertures and now produces vertical-cavity surface-emitting lasers (VCSELs) in the wavelength range 0.85 to 1.3 μm . His best VCSELs require a power of only 50 fJ to transmit one bit and are by far the most energy-efficient in the world for computer interconnects. Thus, the energy hunger of future Exa-Flop supercomputers can be enormously reduced. Bimberg’s VCSEL technologies have also been decisive for developing and demonstrating the world’s first electrically driven single q-bit emitter, a resonant cavity light emitting diode, on the basis of a single InAs quantum dot operating at highest frequencies of 1 GHz.

His patent portfolio covering his most important material and device developments contains about 30 patent families, many of them sold to world market leading companies. Three start-up companies based on such patents have been founded together with his former co-workers. His contributions towards sustainable technologies for a less energy consuming world were recognized in the last few years by bestowing three times the “Green Photonics Award of SPIE” to him and his co-workers in 2012, 2014 and 2015, the Welker-Award and medal in 2015, the UNESCO award in nanoscience and –technology in 2012, his elections as Foreign member to the (US) National Academy of Engineering in 2014 and as Fellow to the National Academy of Inventors in 2016.

Dieter Bimberg has made the fundamental contributions to understanding the growth as well as the electronic and optical properties of semiconductor nanostructures. Moreover, using this fundamental physics base, he has pioneered new electronic and photonic devices in the fields of memories, information science and communications for the benefit of mankind and a sustainable world as a whole.

New Improvements in Nuclear Engineering

by Yassin Hassan, Member EUAS

Short Biography

Professor and Head

Department of Nuclear Engineering

Sallie and Don Davis '61 Professor of Engineering

and Professor of the Department of Mechanical Engineering

Texas A&M University

EDUCATION:

Ph.D., Nuclear Engineering, University of Illinois

Master in Mechanical Engineering, University of Virginia

M.S., Nuclear Engineering, University of Illinois

B.S., Engineering, University of Alexandria, Egypt

FIELDS OF SPECIALIZATION:

Thermal-hydraulics, computational and experimental fluid mechanics and heat transfer, turbulence, two-phase flow, reactor safety, laser-based flow visualization and diagnostic imaging techniques, system modeling and advanced nuclear reactors.

Prior to joining Texas A&M September 1986, he worked for seven years at Babcock & Wilcox Company, where he conducted several thermal hydraulic analyses and undertook development of several computational techniques.

SOCIETY MEMBERSHIPS:

American Society of Mechanical Engineers

American Nuclear Society

American Society for Engineering Education

American Institute of Chemical Engineers

American Institute of Physics

European Mechanics Society

Sigma Xi, The Scientific Research Society of North America

The Honorary Society of Phi Kappa Phi

SPIE-The International Society for Optical Engineering

International Association for Hydraulic Research (IAHR)

International Information Center for Multiphase Flow (ICeM)

Registered Professional Engineer, Texas # 74645

HONORS AND AWARDS:

Fellow of American Association for the Advancement of Science

Fellow of the American Nuclear Society

Fellow of the American Society of Mechanical Engineers

Fellow of International Energy Foundation

2017 James N. Landis Medal of the American Society of Mechanical Engineers for outstanding contribution in nuclear reactor safety through research and education.

2008 American Nuclear Society Seaborg Medal – One of the highest honors of the American nuclear Society (ANS) - The medal named for Glenn Seaborg a Nobel Laureate, recognizes contributions to the peaceful uses of nuclear technology.

2004 Thermal Hydraulics Technical Achievement Award of American Nuclear Society for significant contributions in thermal hydraulics and reactor safety

2003 George Westinghouse Gold Medal Award the of American Society of Mechanical Engineers for Distinguished Achievements and Notable Contribution of the Power Field of Mechanical Engineering

2003 Arthur Holly Compton Award of the American Nuclear Society in recognition of contributions to nuclear engineering education and research
2001 Glenn Murphy Award of the American Association for Engineering Education, "For Outstanding Contributions to the Profession and Teaching of Nuclear Engineering."
1992 Texas Engineering Experiment Station Senior Fellow
1991-1992 Texas Engineering Experiment Station Fellow
1990-1991 Texas Engineering Experiment Station Fellow
Member of the International Nuclear Energy Academy (INEA)
Senior member of American Institute of Chemical Engineers
Akiyama Medal for the best paper at the International Nuclear Engineering Conference (ICONE 24), 2016, (advise Lambert Fick, who the first North American student to receive the Akiyama Medal), 2016.
European Union Academy of Sciences, member, 2016-present.
Certificate of Recognition from the French Nuclear Society for Managing as US Technical Chair of the 9th International Conference on Nuclear Engineering, April 2001
Certificate of Appreciation from Heat Transfer Division of the American Society of Mechanical Engineers on Chairing the Committee on Nucleonics Heat Transfer, 1998-1999.
Certificate of Appreciation at the 7th International Conference on Nuclear Engineering (ICONE-), Tokyo, Japan, April 1999.
Certificate of Appreciation at the 6th International Conference on Nuclear Engineering (ICONE-6), May 1998
DOE Award of Appreciation in Recognition of the Contribution as a Peer Reviewer for FY-2004 Nuclear Energy Research Initiative Grants
Best paper competition at the 19th International Conference on Nuclear Engineering, Osaka, Japan, October 24-25, 2011 (advisee N. Salpeter)
Who's Who in the South and Southwest, Twenty-Second Edition, 1991-1992
Who's Who in America 1992-1993
Who's Who in American Education, 1993
Who's Who in Science and Engineering
Best paper at the ICONE-15, Nagoya, Japan, (advisee Dominguez Ontiveros), 2007
Best Paper at Thermal Hydraulic Session of Young Professionals, ANS Winter Meeting, (advisee Steve Fortenberry), November 2008
Member, Editorial Board of Nuclear Engineering and Design Journal
Theme Editor of Nuclear Energy and Reactors of Encyclopedia of Life Support Systems - United Nations Educational, Scientific and Cultural Organization (UNESCO-EOLSS)
Appreciation plaque for the lecture delivered at the Spring semester seminar at Korea Advanced Institute of Science and Technology, Korea
Guest Professor at Shanghai Jiao Tong University, 2007-present
Adjunct Professor Xi'an Jiaotong University, China, 2013- present.
Member, Editorial Board of the Journal of Energy and Power Engineering in China, Springer.
Member, Editorial Board of Frontiers in Energy, Springer.
Member of the Board of Consulting Editors for the 2010 McGraw-Hill Yearbook of Science & Technology, the companion publication of the McGraw-Hill Encyclopedia of Science & Technology
Member, Editorial Board the Journal of Computational Multiphase Flows
Member, International Advisory Board of several organizations; The University of Tokyo Global COE Program, Nuclear Education and Research Initiative
Associate Editor of Science and Technology of Nuclear Installation Journal
Associate Editor of Journal of Verification, Validation and Uncertainty Quantification
Honorary Chair of the 16th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-16), Chicago, Il., August 30-September 4, 2015
Fellow of European Research Community on Flow, Turbulence and Combustion Society --- This fellowship supported the seminars at the Swiss Federal Institute of Technology (ETH), Zurich and the Paul Scherrer Institute (PSI), Villigen, May 2009.

Elected Member of the Executive Committee of the Nuclear Engineering Division of ASME and of the Executive Committee of the Thermal Hydraulics Division of ANS

Elected Member of the ASME Standard Committee for V&V-30 Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior

Member of the Governing Board of the European Union Thermal-Hydraulics of Innovative Nuclear Systems (THINS) project

Editor of Nuclear Engineering and Design Journal, 2005- 2008

Sworn in 2007 as a part-time Technical Judge, Atomic Safety and Licensing Board Panel (ASLB), US Nuclear Regulatory Commission, Washington DC.

Editor-in-Chief of Nuclear Engineering and Design Journal, 2008-present

EXPERIENCE:

Professor, Department of Nuclear Engineering, Texas A&M University, College Station, Texas, September 1990- present.

Professor, 2003 – present, Department of Mechanical Engineering, Texas A&M University, Joint appointment.

Head and Sallie and Don Davis '61 Professor of Engineering, 2013- present, Department of Nuclear Engineering, Texas A&M University.

Interim Head, 2012-2013, Department of Nuclear Engineering, Texas A&M University

Adjunct Professor 2009 – present, The University of Texas of the Permian Basin.

Associate Head, 2002 - 2012, Department of Nuclear Engineering, Texas A&M University.

Graduate Program Coordinator, September 1990 - 2002, Department of Nuclear Engineering, Texas A&M University.

Visiting Researcher, Division of Systems Research, Office of Nuclear Regulatory Research, US Nuclear Regulatory Commission, Rockville, MD, June - August 1995. Review, analysis and assessment of thermal hydraulic codes for advanced nuclear reactor designs.

Visiting Professor, The Summer School of J.M. Burgerscentrum, Delft University of Technology, The Netherlands. Summer 1995. Lectured on the use of Imaging Techniques including Particle Image Velocimetry in two-phase flows.

International Atomic Energy Agency (IAEA) Expert, Reactor Engineering Division, Jozef Stefan Institute, Ljubljana, Slovenia, June 1994. Responsibilities included a project on upgrading of Krsko Nuclear Power Plant (IAEA Project No. SLO/9/002) and reviewed the methods and results of several design bases and accident analyses performed at Jozef Stefan Institute.

Associate Professor, Department of Nuclear Engineering, Texas A&M University, College Station, Texas, September 1986 - August 1990.

Principal Engineer, Nuclear Power Division, Babcock & Wilcox Company, Virginia, 1984-1986

Senior Engineer, Nuclear Power Division, Babcock & Wilcox Company, Virginia, 1982- 1984.

Engineer, Nuclear Power Division, Babcock & Wilcox Company, Virginia, 1980-1982.

Research Assistant, Department of Nuclear Engineering, University of Illinois, 1974-1979.

PUBLICATIONS:

According to the science Citation Index, publications authored or coauthored by Y.A. Hassan have been cited more than 3473 times (h-index=28, i10-index =75).

Number of refereed Journal publications: 155

Number of refereed papers and conference proceedings: 281

Summaries in Transaction: 347 Number of Reports: 32

Editorships: 55 Chapters in books: 8

Keynote Addresses, Invited Speaker or Seminar Speaker: 110

The number of ANS summaries authored by his students and him are more than 300 summaries (the largest for any ANS member since the establishment of the American Nuclear Society in 1950).

He is Professor and Head of the Department of Nuclear Engineering, Sallie and Don Davis'61 Professor of Engineering and also Professor of the Department of Mechanical Engineering at Texas A&M University. Prior to joining Texas A&M September 1986, he worked for seven years at Nuclear Power Division, Babcock & Wilcox Company, Lynchburg, Virginia. His research is in computational and experimental thermal hydraulics, reactor safety, laser-based flow visualization and diagnostic imaging techniques, system modeling, multiphase flow, transient and accident analyses and advanced nuclear reactors.

He is a fellow of American Association for the Advancement of Science (AAAS), a fellow of American Nuclear Society (ANS) and a fellow of American Society of Mechanical Engineers (ASME), and awarded 2008 American Nuclear Society Seaborg Medal (this award recognizes an individual who has made outstanding scientific or engineering research contributions to the development of uses of nuclear energy), 2003 George Westinghouse Gold Medal award (distinguished achievement in and notable achievements in power field of mechanical engineering), 2004 Thermal Hydraulics Technical Achievement award (highest award given by Thermal Hydraulic Division of ANS in recognition of outstanding technical achievement), 2003 Arthur Holly Compton Award of the American Nuclear Society in recognition of contributions to nuclear engineering education and research, 2001 Glenn Murphy award of the American Association for Engineering Education and 2017 James N. Landis Medal of the American Society of Mechanical Engineers in recognition of outstanding contribution in nuclear reactor safety through research and education. *He is the editor-in-chief of the premier Nuclear Engineering and Design Journal.*

He supported NRC's research division activities in certification of AP600, and participated in the PIRT panel of high temperature gas cooled reactors and ARC700 CANDU reactor. He serves as a technical expert for the International Atomic Energy Agency, national laboratories and a number of other technical review panels. He has served as adjunct professor at several international universities. He serves as a member of the governing board of the European Commission Consortium of the thermal hydraulics of innovative nuclear system project and a member of international advisory board of the Korea Atomic Energy Research Institute (KAERI), Korea. Member of the Advisory Council of the Department of Nuclear Engineering, University of Tennessee and chair of the review committee of the department. External reviewer of several nuclear engineering programs: University of McMaster, Canada; Seoul National University, Korea; Royal Institute of Technology, Sweden; Academy for Global Nuclear Safety, Tokyo Institute of Technology.

He has authored more than 440 refereed publications in technical journals and conference proceedings (154 technical journals and 286 conferences) and 345 summaries in ANS Transactions (the largest for any ANS member since the establishment of the American Nuclear Society in 1950). *Dr. Hassan was sworn in 2007 as a part-time technical judge to the Atomic Safety and Licensing Board Panel, US Nuclear Regulatory Commission.*

New developments in Nanomagnetism

by Hartmut Zabel, Member EUAS

Short Biography

Education/Degrees:

1969 Bachelor in Physics, University of Bonn
1973 Master in Physics, Technical University of Munich
1978 Ph.D. in Physics, University of Munich

Academic Positions:

1978 - 1979 Postdoctoral Fellow, Department of Physics, University of Houston, Texas
1979 - 1983 Assistant Professor of Physics, University of Illinois at Urbana - Champaign
1983 - 1986 Associate Professor of Physics, University of Illinois at U - C
1986 - 1989 Professor of Physics, University of Illinois at U - C
1989 - 2013 Chair, Professor of Experimental Physics/Solid State Physics, Ruhr-Universität Bochum
2013 – 2019 Visiting Senior Research Professor, University of Mainz
since 1.4.1989 Adjunct Professor of Physics, University of Illinois at U - C

Guest positions:

Summer Guest Scientist, Brookhaven National Laboratory, 1985 and 1988; Guest Scientist, Risø National Laboratory, Denmark, 1986; Guest Scientist of the NIST, Reactor Division, Gaithersburg, USA, 1993; Guest Scientist of the Institut Laue-Langevin, Grenoble, France, 1997; Guest Scientist and Lecturer, University of Uppsala and KTH Stockholm, Sweden, 1998/99; Senior Guest Research Professor, University of Mainz, Germany, since 2013.

Fellowships/Awards:

Fellow of the Cusanus Fellowship Program for Superior Students, 1971 – 1973; Fellow of the Institute for Advanced Studies, University of Illinois at Urbana-Champaign, 1982; Fellow of the JSPS, 1989; Fellow of the Volkswagenstiftung, 1993 and 1997; Election to Fellow of the APS, 1996; Honorary Doctor of the KTH Stockholm, 2001; Elected “Outstanding Referee” of the APS, 2010; MAINZ Research Award, J G University Mainz, 2013; Elected Member, European Academy of Sciences, 2017.

Research Networks, Panels, and Advisory Committees:

Department of Energy (DOE) Program Director in the Materials Research Laboratory for the Condensed Matter Science Program (1986 – 1989); Member of the US DOE review panel “HFBR - Neutron Beam Lines” (1988); Member, Basic Energy Sciences Advisory Committee of the US DOE (1992); Chair, German – Russian Collaboration “Advanced Materials with Collective Electronic Properties”, funded through the DFG and the Russian Academy of Science (1992-2002); Chairman of the DFG Collaborative Research Center “Magnetic Heterostructures: spin structure and spin transport” (2000-2011); International Advisor of the project “Fundamental Research and Applications of Magnetism” University of Uppsala (2001-2006); Chairman, Scientific Council of the Swiss Intense Neutron Source (SINQ) (2003-2005); Member, Beam time committee, BESSY Synchrotron facility, Berlin (2005-2012); Member and Chair of the Scientific Council, Institut Laue-Langevin, Grenoble (2006-2010); Member, Scientific Advisory Committee of the Hahn-Meitner Institut, Berlin (2004-2008); Divisional Associate Editor of the journal *Physical Review Letters*, (2012-2018); etc.

Further professional activities

Advisor of 50 PhD students with successful thesis completion, referee work for more than 25 journals, referee for more than 15 funding agencies, member of numerous national and international PhD disputation panels, organization of 4 international conferences and 4 summer schools, member of numerous advisory boards of national and international conferences, Chief Editor of the Elsevier Journal: *Superlattices and Microstructures*, Elsevier (2003-2013); etc.

Publications:

More than 500 refereed papers in technical journals, 36 review papers and book chapters, editor of five books, author of the textbook “Physik”, Thieme publisher, 1st edition 2011, 2nd edition 2016, author of the textbook “Medical Physics”, de Gruyter publisher, 1st edition 2017.

Research activities:

Hydrogen in metals, graphite intercalation compounds, semiconductor heterostructures, metal superlattices and heterostructures, diffusion in solids, oxidation of epitaxial metal films, phase transitions, magnons, phonons, magnetism of thin films and heterostructures, proximity effects between superconductors and ferromagnets, spintronic materials, nanofluidics, magnetic x-ray and neutron scattering, magneto-optics. Spin-ice, magnetic nanoclusters, odd-triplett superconductivity; Most recently: time-resolved magnetization precession and magnetization reversal processes, antiferromagnetic spintronics.

My research interests are in condensed matter physics, including phenomena such as phase transitions, lattice vibrations, self-diffusion, magnetism, and superconductivity. In addition to specific research projects, it was always important for me to develop new instrumentation and share this with interested groups. In this respect we have developed an instrument for polarized neutron reflectivity at the research reactor HFR of the Institute Laue-Langevin, Grenoble, France [1], and a chamber for resonant magnetic x-ray scattering and spectroscopy at the synchrotron facility BESSY II of the Helmholtz Zentrum, Berlin, Germany [2]. Furthermore, we have developed the magneto-optical Kerr effect in such a way as to gain magnetization vector information at higher order diffraction peaks of laser light scattered from patterned magnetic nanostructures [3]. My current research interest is focused on antiferromagnetic spintronics, which is described in some more detail as follows.

Any second we generate trillions of data that need storage and accessibility for further processing. In the past information storage was achieved mainly by ferromagnetic mass storage devices: magnetic core memory, magnetic tapes, and hard disks. To handle the increasing demand for big data storage and manipulation, new concepts are required. One promising approach is the use of antiferromagnets instead of ferromagnets for their operational speed is a factor 1000 higher. In ferromagnets the local magnetic moments are aligned parallel by exchange coupling and crystal anisotropy. As the size of ferromagnetic domains decreases, they become increasingly wobbly fighting against thermal fluctuations. Each ferromagnetic domain on a hard disk represents one bit. So, decreasing the domain size increases the storage density. In our present day TB hard disks one ferromagnetic has the size of only a few nanometers. Antiferromagnets, in contrast, with staggered magnetic moments (Figure 1) have no size limitation. Therefore the voxel volume can be decreased further without loss of information. Moreover, antiferromagnets are insensitive to external magnetic fields, providing a much more robust storage than ferromagnets. Furthermore, the intrinsic operational frequency is in the terahertz regime instead of gigahertz for ferromagnets, i.e. a factor of 1000 higher. All this calls for a closer inspection of antiferromagnets as potential information storage media of the future [4,5].

The existence of antiferromagnets was predicted by Louis Néel (Physics Nobel Laureate 1970) on the grounds of suspicious magnetic properties of some materials. But the antiparallel spin structure was not confirmed until Clifford Shull (Physics Nobel Laureate 1994) showed by early neutron scattering work the existence of an extra magnetic Bragg reflection that signals the staggered antiferromagnetic spin order. Since then antiferromagnets converted from exotic materials to an increasingly important player in nanomagnetism, spintronics, and information technology. The term “spintronics” stands for electronics with the spin as an additional degree of freedom for controlling charge currents in metals and semiconductors via magnetic fields in addition to electric fields. However, up until recently the role of antiferromagnets in spintronics was still more of a chaperon type: in sandwich structures consisting of stacked Ferromagnetic /

antiferromagnetic layers with common interfaces, antiferromagnets do not contribute of the magnetization, but they control the magnetization reversal mechanism of the neighboring ferromagnetic layers. Only recently antiferromagnets themselves have entered center stage. The perspectives are promising [6].

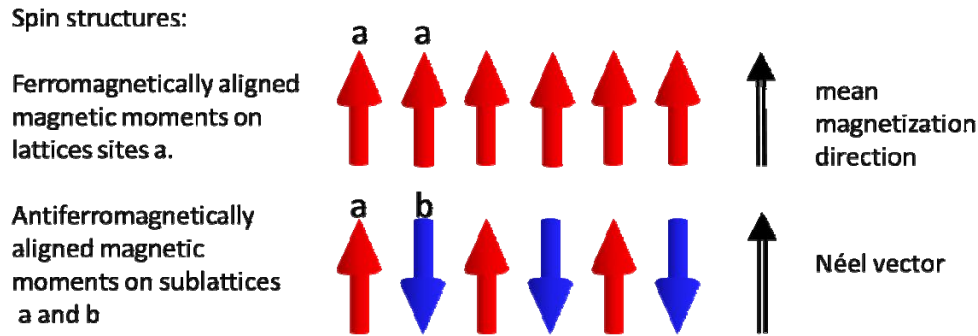


Figure 1 – Spin structure of ferromagnets and antiferromagnets. In ferromagnets all magnetic moments within a domain are parallel contributing to the overall magnetization of a material and defining the mean magnetization direction. In antiferromagnets neighboring magnetic moments are oriented antiparallel on sublattices a and b. The Néel vector defines the orientation of the staggered magnetic moments, whereas the mean magnetization is zero.

Many years of extensive research in nanomagnetism have affirmed that magnetic domain size and magnetic domain walls in ferromagnets can be controlled and manipulated by external and internal parameters such as shape and aspect ratio of magnetic islands, magnetic anisotropy, and exchange coupling to an adjacent antiferromagnetic layer. Domain wall motion and magnetization reversal can be achieved not only by external magnetic fields but more effectively by spin torque that a spin current transfers to the magnetization with opposite orientation. Control over domain size, domain walls, and over magnetization reversal is essential for the operational capabilities of ferromagnets in information technology [7,8,9]. For the groundbreaking ideas of ferromagnetic spintronics Albert Fert and Peter Grünberg received the Physics Nobel prize in 2007. The main concepts that have spurred ferromagnetic spintronics to an unprecedented success need to be reinvented for antiferromagnets.

What is considered the main incentive for the development of antiferromagnetic spintronics turns out to be - at the same time - the biggest obstacle. Antiferromagnets can only be used for information storage if data can be stored and retrieved without loss. The main question is: how?

Antiferromagnets do not feature an intrinsic domain size nor can the domain size be manipulated by external magnetic fields. Furthermore, to reorient the Néel vector of the staggered magnetization (see Figure 1), magnetic fields of several Tesla are required, beyond any reasonable practicality in spintronics. Therefore different means of manipulation have to be invented. This could be either elastic strain, laser pumping, or an electric current. Present day research explores all three avenues.

Like ferromagnets, antiferromagnets show crystal anisotropy, meaning that the crystal lattice reacts on the orientation of the Néel vector. This indicates that the crystal lattice is sensitive to the orientation of unfilled and uncompensated orbitals of atoms that carry spin and orbital magnetic moments. In ferromagnets crystal anisotropy is important, but it is

only one contribution to magnetic anisotropy. The others are shape anisotropy depending on size and aspect ratio of magnetic islands, surface anisotropy dominating in very thin ferromagnetic films, and uniaxial anisotropy stemming from interfaces. In antiferromagnets all the other anisotropies drop out and only the crystal anisotropy remains, signifying its importance and indicating strategies for strain control over antiferromagnetic domains [10].

Other strategies for antiferromagnetic domain manipulation use femtosecond laser pulses for creating a transient ferromagnetic state that can be controlled by proven ferromagnetic methods for domain manipulation [11,12]. Even unpolarized electric current pulses have been shown to switch domains in some antiferromagnetic materials [13].

It is not trivial to get information on the Néel state of antiferromagnetic thin films. Neutron scattering would be the most suitable method, but fails due to intensity limitations when decreasing the sample size to the nanometer scale. However, x-ray absorption spectroscopy using linear polarized synchrotron radiation turns out to be extremely useful for studying antiferromagnetic properties. The method is coined *x-ray magnetic linear dichroism*. The electric field vector of x-rays is sensitive to the orientation of molecular orbitals in antiferromagnets. So, two x-ray spectra with perpendicular electric field vectors sensing the transition from core levels to the Fermi energy will show subtle but characteristic differences. This difference can be related to the Néel vector in antiferromagnetic domains. As mentioned before, antiferromagnetic domains turn out to be rather small on the nanometer scale. An x-ray beam with a footprint on the micrometer scale will take a statistical average of antiferromagnetic domains that populate domains with different Néel vectors. In case of equal population, the difference spectrum vanishes. If manipulation of antiferromagnetic domains succeeds, one domain orientation will dominate over the other and this will be visible in the difference absorption spectrum. Figure 2 shows an example of x-ray absorption spectroscopy on the antiferromagnet Mn_2Au , which is considered to be one of the most favorable candidates for antiferromagnetic spintronics because of its metallic conductivity. Most other antiferromagnetic materials are insulators. In Figure 2 one can recognize that the application of strain indeed leads to a reorientation of antiferromagnetic domains, resulting in characteristic peaks at the absorption maxima of the L_3 and L_2 edges of Mn ions in Mn_2Au .

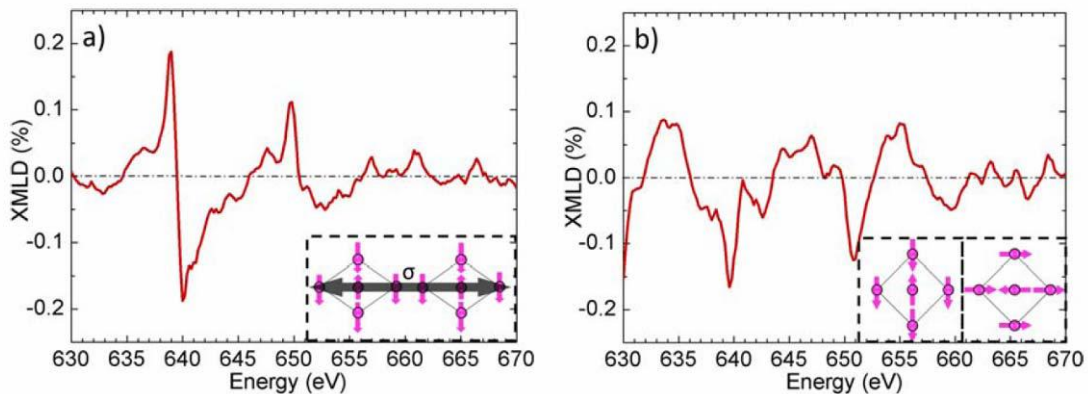


Figure 2 – Difference x-ray absorption spectra recorded with linear polarized x-rays signaling any orientational difference of antiferromagnetic domain population. The spectra are taken at the manganese L_3 and L_2 in the antiferromagnet Mn_2Au . The spectra are measured for strained (a) and unstrained (b) Mn_2Au

layers. In the unstrained case the signal is on the 0.1% level is attributed to noise. The inset in (a) sketches the magnetic moment configuration in the strained sample with stress σ (gray arrows) and elongation along one remaining Néel vector orientation. The inset in (b) sketches the magnetic moment configuration of an unstrained sample with two equivalent antiferromagnetic domains with Néel vectors pointing in two orthogonal directions. From Ref. 14.

By the same token one may also use a finely focused linear polarized x-ray beam for scanning over the sample surface. In resonance mode, photoelectrons will be released that can be detected by a photoelectron detector. This microscopic method is known as photoemission electron microscopy (PEEM). The photoelectron yield depends on the orientation of the linear polarized x-ray beam, signifying differently oriented antiferromagnetic domains. With PEEM antiferromagnetic domains can be imaged directly. In our present work we use x-ray absorption spectroscopy (XAS) with linear polarized synchrotron radiation as well as PEEM imaging of antiferromagnetic domains in response to elastic strain, electric current, and in the future also in response to femtosecond laser pumping. With this work we hope to contribute to a deeper understanding of what controls antiferromagnetic domain size and how domain size and domain orientation can be externally controlled by various unconventional mechanisms.

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Recent Advances in Theoretical Chemical Physics

by Antonio Varandas, Member EUAS

Short Biography

A.J.C. Varandas received a diploma in Chemical Engineering from the University of Oporto (Portugal), and a Ph.D. in Theoretical Chemistry from the University of Sussex (U.K.) under the direction of Professor John N. Murrell.

After graduation in Oporto, he joined the staff at the Department of Chemistry of the University of Coimbra as Assistant Professor, where he occupies since 1988 a position of Full Professor and directs the group of Theoretical & Computational Chemistry. In 1988, he was Invited Professor and Visiting Research Scholar of Minneapolis Supercomputer Institute at the University of Minneapolis (USA) and, from June-July 1995, Cherry L. Emerson Fellow at the Department of Chemistry of Emory University in Atlanta (USA).

In 2009, he was awarded a Visiting Professorship for Senior International Scientists from the Chinese Academy of Sciences. His research interests cover a wide range of topics in theoretical chemistry from potential energy surfaces to non-adiabatic effects in ro-vibrational spectroscopy and reaction dynamics. Some of his studies have implications on theoretical environmental chemistry, particularly in combustion chemistry and issues related to the ozone chemistry at the middle atmosphere.

He has 400 research papers in those areas, and co-authored a monograph entitled Molecular Potential Energy Functions (Wiley, 1984). Edited special issues of Physica Scripta (IOP, 2011), and Advances in Physical Chemistry (Hindawi, 2012), and co-edited a book in memorial of Ruy Couceiro da Costa (Universidade de Coimbra, 2011). Wrote 2 books and 2 books of lectures notes, all in portuguese, devoted to Computational Methods, Quantum Chem-istry, and Statistical Mechanics.

Oriented 30 PhD students from various nationalities, including Brazil, China, Cuba, India, Italy, Moldavia, Portugal, and Spain. Received the following awards: "Artur Malheiros" Prize for Physics and Chemistry of the Lisbon Academy of Sciences (1985); "Ferreira da Silva" Prize of the Portuguese Chemical Society (1991); Prize Stimulus to Excellence of the Portuguese Ministry of Science, Innovation and High Studies (2004).

Received honorific titles from Instituto Superior de Tecnologias y Ciencias Aplicadas (La Habana, Cuba, 1998), Dalian Institute of Chemical Physics (Dalian, China, 2005), and Henan Normal University (Henan, China, 2006). In 2006, he was elected corresponding member of the Lisbon Academy of Sciences. Also, in 2015 he was elected member of the EU Academy of Sciences.

Potential Energy Surfaces & Reaction Dynamics within the Born-Oppenheimer Approximation and Beyond

My research interests have long focused on theoretical studies of molecular systems, covering both energetic and dynamics aspects. In addition to fundamental research, I have also been involved on the application of theoretical methods to specific systems of practical interest. Some recent examples of the progress that I and my collaborators have made on specific problems during the past few years are highlighted in the following paragraphs. Inescapably, emphasis will be given to the author's own work, with assess to

other publications possible via crossreferencing within the cited literature.

The BO Approximation: Validity, Implications & Generalization

At that occasion of celebrating its 90 years, it is appropriate to begin with the Born-Oppenheimer (BO) approximation which treats the motions of electrons and nuclei as separable. First, we assessed its validity [1] by considering dipositronium and allowing the mass of the two involved positive fermions (positrons) to vary such as to reach the proton mass or even reach infinity, thus allowing the BO approximation to be exact.

Due to separating the motions of the light and heavy particles, the BO approximation brings with it important topological implications. Consider the case of a molecule with N nuclei, thence a PES with $3N-6$ nuclear degrees of freedom (DOF). It is well established that such a PES may conically intersect another of the same spin and spatial symmetry along a locus of $3N-8$ dimensions. We refer to the two conically intersecting electronic states as defining a 2D Hilbert space. Assume now that wave function of one of the two electronic states is transported adiabatically along a loop that encircles the crossing locus. In this case, Longuet-Higgins has topologically demonstrated that the wave function will change sign when closing the loop [2]. This happens irrespective of the adiabatic electronic state of the 2D HS where the wavefunction is adiabatically transported in configuration space. More intricate conical crossings may arise for polyatomics larger than triatomic. In the past few years we have considered the cases of 2D, 3D, 4D, and 5D HS of electronic degeneracy. First, we have shown that in the case of a 2D HS, the change of sign along the above loop in configurational space is equivalent to the sign change in rotating the adiabatic electronic state by π in the 2D function space defined by the two diabatic electronic states. Furthermore, we have demonstrated by reduction ad absurdum that for higher dimensionality HS, only two states show such a sign change, indeed for the innermost conical pair [3].

Electronic Structure: Potential Energy Surfaces, CBS Extrapolation, WF-based vs DF-based Approaches

The electronic problem is next addressed, with recent progress surveyed on the extrapolation to the complete basis set limit [4,5] of the energies calculated pointwise from the corresponding Schrödinger equation. Although extrapolation schemes for the Hartree-Fock energy have also been considered [6], the focus has been on the much slower convergent, and computationally demanding, correlation energy. Because quantum chemistry calculations are frequently based on the gold standard coupled cluster theory with single, double, and perturbative triple excitations, CCSD(T), which is often affordable only for relatively small molecules with the smallest basis sets, single-level extrapolations from one raw energy were also investigated as they could attain maximum usefulness for larger systems [7]. Whenever possible, raw data from second-order MÖller-Plesset perturbation theory, as well as CCSD, CCSD(T), and multireference configuration interaction methods are utilized.

Most recently, we have put into perspective the methods of quantum chemistry used to study many- vs few-atom molecular potentials. With the rule of thumb being Kohn-Sham density functional theory (DFT) for the former, wave-function (WF) based methods for the latter, such a dichotomy is mostly attributed to cost-effectiveness. This led us to compare

and contrast the energetics and time performances of DFT vs WF-based methods for a vast number of reactions and isomerizations. Strikingly, a cost-effective wave function-based MÖller-Plesset perturbation-theoretic (MP2) method combined with CBS extrapolation from the first steps, (d,t) or just d or t, of the hierarchical staircase is then shown to rival with Kohn-Sham density functional theory both accuracy- and time-wise [8]. The energies so obtained may then be given the quality of couple-cluster type via a variable-scaling opposite spin method [9].

Strategies for global representation of the potential energy surfaces have also been pursued, based on the modern partition of the correlation energy into its static and dynamic components, followed by a many-body expansion of the associated energies. The advantageous approach consists therefore of developing the energy as a double many-body expansion (DMBE), thus treating both Hartree-Fock and correlation contributions (preferably after CBS extrapolation) as separate MBEs [9]. Having its foundation many years ago, the purpose of the novel scheme called Combined Hyperbolic Inverse-Power Representation [10] is to construct such a physically motivated development such as to make best suited to fit output energies from ab initio electronic structure codes. Having also suggested a scheme to model multi-sheeted PESs (showing conical intersections), we have also suggested a way to embed cusp-like behavior into single-sheeted forms for triatomic species [11]. As a case study, the challenging ground-state C_3 has been considered, which has four conical intersections due to combined Jahn-Teller plus pseudo-Jahn-Teller interactions [12]. Such work is currently progressing on C_4 and even larger carbon clusters.

Quantum Reactive Scattering

The accurate solution of the nuclear Schrödinger equation for triatomic reactions on a single Born-Oppenheimer (BO) PES was pioneered by Kuppermann and collaborators, with various theoretical methods suggested ever since: R-matrix propagation, use of hyperspherical coordinates, S-matrix formulation, and others based on the Newton variational-principle. Significant advances on measurements of differential cross-sections of triatomic reactions fuelled theoretical progress leading to further developments of both time-independent and time-dependent approaches. In particular, Billing and Markovic formulated the 4D quantum mechanical problem of triatomic reactive scattering using hyperspherical coordinates to perform 3D as well as coupled 3D wave packet calculations of the $D+H_2$ prototypical reaction in the simplest cases of $J=0$, and $J=1$. In 2013, Adhikari and Varandas [13] extended such a formalism to carry out time-dependent wave packet calculations for $J=0$ as well as $J\neq 0$. More recently, Adhikari and coworkers implemented the OpenMP-MPI parallelized algorithm to investigate the workability of the time dependent wave packet approach on the D^++H_2 system both using the lowest adiabatic singlet sheet (1^1A) [14] as well as the lowest three singlet sheets (1^1A , 2^1A and 3^1A) [15] of the DMBE PES [15] for H_3^+ . State-to-state as well as total cross-sections and rate coefficients calculated therein have shown good agreement with the corresponding experimental measurements and previous calculations [16]. The method has most recently been applied to the $O+OH\rightarrow H+O_2$ reaction [17] using the approximate J-shifting scheme for estimating $J\neq 0$ attributes. Being one an important prototypical exothermic reaction occurring without a barrier, progress is now directed towards its reverse reaction which is known as the most important reaction in combustion.

Exploring a Simplified Treatment of Attosecond Quantum Photodynamics

The interaction of a laser field with atoms and molecules leads to nonlinear nonperturbative processes both of practical and fundamental interest in strong field science. Among them, high-order harmonic generation (HHG) is key in strong field physics, although not yet established as a practical tool to probe the structural dynamics of polyatomic molecules. HHG spectroscopy is commonly understood within the three-step model: an electron tunnels out of the parent atom or molecule and recombines with the parent or neighbouring ion at the end of the laser driven motion, leading to emission of high-energy radiation which extends to the UV and X-ray regions. In fact, HHG spectroscopy exploits the correlation between the nuclear wave packet created in the cation and the electron wave packet to measure the nuclear dynamics on a sub-femtosecond time scale. Inspired by recent experimental work and our own theoretical [18-20] work to achieve vibrational dynamics in simple molecules, we are currently developing efforts to study the photodynamics of polyatomic molecules due to strong field ionization, yet in a simplified manner which implies the use of severe assumptions. For example, we have been studying the fast rearrangement in CH_4^+ from its initial Td structure to equilibrium C_{2v} under the assumption that the dynamics of the electron can to some extent be ignored. Despite such a drastic assumption, the predictions agree well with the experimental results. Such dynamics studies use extensive ab initio calculations for characterizing both the ground and excited states of the molecule and its cation. Specifically, after rationalizing the ab initio results, a model Hamiltonian is constructed, which includes both the ground and one or more excited states potential energy curves of the cation. Photoelectron spectra of molecule and its deuterated counterpart are then calculated and compared with the available experimental results. The HHG signals due to the strong field ionization of are subsequently calculated from the autocorrelation functions, and the results compared with available experimental and theoretical ones.

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