EU ACADEMY OF SCIENCES

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EU ACADEMY
2020 ANNUAL REPORT

The President of EUAS

Professor E.G. Ladopoulos

& The Board Governors of EUAS

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About an Energy World by the Theory of "Universal Mechanics" Is That Possible ?

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 400 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.
High Index by Google Scholar.
President & CEO of the EU Academy of Sciences.
Member by several Academies in USA.

For the design of the future spacecraft of any speed, the very groundbreaking theory of ***"Universal Mechanics"*** is proposed and investigated. 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. Also, 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. Thus, for the future 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 future spacecraft will be moving by using laser engines.

After the speed of light an energy world would appear. Is that possible ? Yes of course it is possible. Over the past many people have seen in the sky several lights in the form of spacecraft or flying saucers. So, these might be aliens much more developed than humans with their science very much developed and their spacecraft is in energy form. Thus, if the spacecraft exceeds the speed of light, then it becomes an energy spacecraft. In that case an Energy World would be possible.

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 future 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.

One more question is the following: What happens with our theory if somebody in the very future proves that the speed of light is not the maximum speed in the whole universe, but there is another type of energy with higher speed ? The answer is that our theory of "Universal Mechanics" will valid over the centuries and the milleniums, as the spacecraft when reaching the speed of light then becomes energy and will not be mass any more. Consequently, after the speed of light there is no mass available, but only energy. According to NASA the Large and Small Magellanic clouds were thought to be the closest galaxies to ours, until 1994, when the Sagittarius Dwarf Elliptical Galaxy (SagDEG) was discovered. In 2003, the Canis Major Dwarf Galaxy was discovered - this is now the closest known galaxy to ours. So, The Canis Major Dwarf Galaxy is only 25,000 light years from the Sun, and 42,000 light years from the Galactic center. It too, is well-hidden by the dust in the plane of the Milky Way - which is why it wasn't discovered until recently. To get to the closest galaxy to ours, the Canis Major Dwarf, at Voyager's speed, it would take approximately 749,000,000 years to travel the distance of 25,000 light years! If we could travel at the speed of light, it would still take 25,000 years. On the other hand, the galaxy MACS0647-JD appears very young and is only a fraction of the size of our own Milky Way. The galaxy is about 13.3 billion light-years from Earth, the farthest galaxy yet known, and formed 420 million years after the Big Bang. The universe itself is only 13.7 billion years old, so this galaxy's light has been traveling toward us for almost the whole history of space and time.

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: $$\sigma_{21}^{0} = \sigma_{12}^{0}, \sigma_{31}^{0} = \sigma_{13}^{0}, \sigma_{32}^{0} = \sigma_{23}^{0} \quad (2)$$

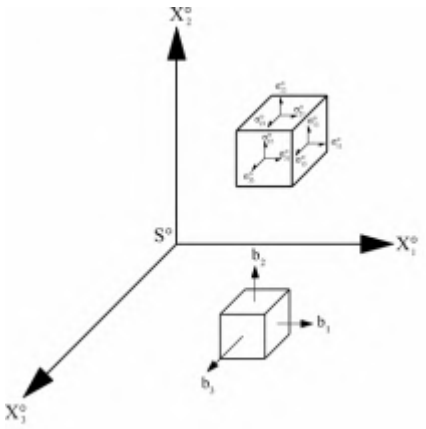

Fig. 1 The state of stress σ_{ik}^{0} in the stationary system S^{0}.

In addition, we consider an infinitesimal face element df with a directed normal, defined by a unit vector **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:

$$\mathrm{d}\boldsymbol{\sigma}(\mathbf{n}) = \boldsymbol{\sigma}(\mathbf{n})\,\mathrm{d}f \quad (3)$$

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

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

where 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).

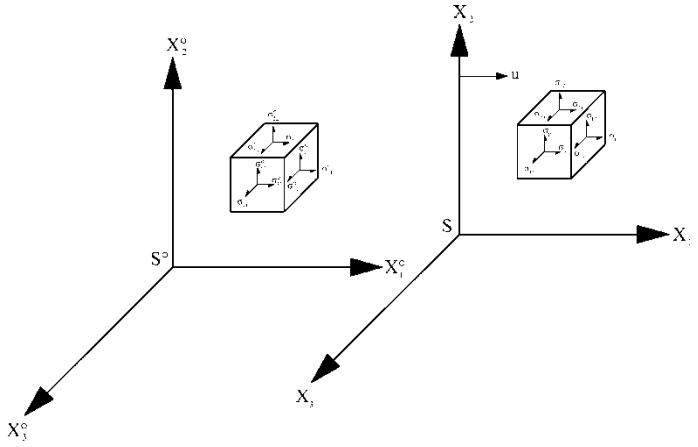

Fig. 2 The state of stress σ_{ik}^{0} in the stationary system S^{0} and σ_{ik} in the airframe system with velocity u parallel to the x_1 - axis.

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

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

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.

Beyond the above, consider the general system of continuously matter, inside which invisible heat conduction can take place. Then the momentum density $\mathbf{g}$ of this system is given by the ***Universal Equation of Thermo-Elasticity:***

$$\mathbf{g} = m\mathbf{u} + \frac{(\mathbf{u},\boldsymbol{\sigma})}{c^2} + \frac{\boldsymbol{\xi}}{c^2} \tag{8}$$

in which $\mathbf{u}$ denotes the velocity of the matter at the place and time considered, $\boldsymbol{\sigma}$ the relative stress tensor, $m = E/c^2$ is the total mass density and $\boldsymbol{\xi}$ is given by:

$$\boldsymbol{\xi} = \gamma\left[\mathbf{V} - \mathbf{u}(\mathbf{V},\mathbf{u})/c^2\right] \tag{9}$$

with $\mathbf{V}$ the four vector.

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 the current author. Hence, by the current author is completed the theory of Albert Einstein for the whole universe regarding mechanics engineering behavior.

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 3*c*/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 future 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.

The **Universal Stress Intensity Factors** are given by the formulas:

$$K_I = \lim_{x_1 \to 0} \left\{ \sqrt{2\pi x_1}\, \sigma_{22}^0 \right\} \tag{10}$$

$$K_{II} = \lim_{x_1 \to 0} \left\{ \sqrt{2\pi x_1}\, \gamma \sigma_{12}^0 \right\} \tag{11}$$

$$K_{III} = \lim_{x_1 \to 0} \left\{ \sqrt{2\pi x_1}\, \sigma_{23}^0 \right\} \tag{12}$$

Hence, from eqs (10) to (12) follows that 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. So, because of the above difference of the stress intensity factors, follows that the fracture behavior of the future spacecraft would be much different and thus special materials should be used for their construction.

When the relative stress intensity factors are taken into consideration the whole theory is known as ***"Universal Fracture Mechanics".***

Covid-19 Evolution Analysis at Madrid and Andalusia, Spain by Differential Equation Model

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.

Abstract

Since the beginning of the COVID-19 pandemic, the concern about the SARS-CoV-2 virus spread is growing. Decision takers require affordable tools that provide strategic information regarding the effectiveness of containment measures. These may range from the suspension of the educational activity to different strictness of lockdown periods. The source of information to feed such tools should be simple and accessible. In this line, this work considers the mortality curve as a downsized and time-shifted footprint of the generally undetermined, real infection curve. Even if the scale between both curves is unknown, their shape allows obtaining characteristics of the spread dynamics. This, in turn, provides information on the infected fraction of the population at a given time.The number of parameters to fit the model from the mortality curve has been minimized so the method is flexible enough to face disrupted input data, usual during a disease outbreak. Once these parameters are obtained, the model predicts the evolution of the mortality and infected cases curves. This allows to evaluate the possibility of a rebound after lifting population containment (lockdown) measures. Two cases illustrate the application of the model to the COVID-19 outbreak: The Spanish autonomous communities of Madrid and Andalusia. Madrid is an example where the virus spreads rapidly, while Andalusia reflects slower growth. Results show the evolution of the infected fraction of the population reaching between 52% and 12% for Madrid, and between 6% and 2,5% for Andalusia, in connexion with an *IFR* between 0.008 and 0.0025 (Infection-Fatality Rate). It also predicts the very different effects from a total lift of the lockdowns: from 1 to 3 deaths per 10 000 inhabitants in the

case of Madrid, to 15 deaths per 10 000 inhabitants in Andalusia. The case of Andalusia also indicates the possibility of a rebound. Even maintaining the lockdown, if any relief attempt leads to relevant social connectivity, a steep increase can be triggered. The economic burden of the lockdowns induces lifting confinement. In this case, strategies making relevant sanitary differences for different age intervals seems the only way to reduce the commented numbers. This work offers some suggestions. The use of this easily understandable model provides strategic insights for governments and contributes to optimizing disease management. The reasonable skills needed and the simplicity (non-intricacy) of the model also allows minimal costs, which are beneficial for rapid and/or low resource assessments (i.e. developing countries). The use of the tool in combination with blind antigen and antibody response testing to double-check critical parameters is encouraged.

1. Introduction

The Coronavirus Disease 19 (COVID-19) is a recent global pandemic [1] counting with 3 635 509 cases and 251 585 deaths worldwide by May 5th, 2020 [2]. This worldwide outbreak seems to impact deeply world's economy and social welfare [3]. Thus, governments and decision-makers are focused on effective strategies to cope with COVID-19 spread. The main strategies applied by governments are (1) general population quarantine (or lockdown), (2) isolation, and (3) social distancing [4], [5]. However, the worldwide outbreak of COVID-19 has shown a heterogeneous landscape in decision-makers criteria and measures. In addition, several attempts to understand the spread of COVID-19 aim to establish evidence-based recommendations. Some preliminary models established early infection rates [6]–[8], while more sophisticated models came afterward, applying statistical [9], [10], and non-statistical [11], [12] frameworks. However, data reliability seems questionable and needs to be considered. Two probable causes can be drawn: (1) scarcity of data, and (2) unexplored influential factors, e.g., derived infections [13] or neurological syndromes [14]. Thus, a parsimonious mathematical model (i.e., a simple model with relevant explanatory predictive power) can help in this scenario.

This paper proposes a parsimonious model for COVID-19 spread and applies it to available data from Spain. For maximizing the reliability of available data, the mortality curve is used as input instead of contagion or infection. Infection curves have additional distortion sources like (i) availability of tests and (ii) development of symptoms. Currently, tests are scarce and not applied widely [15], [16], and there is a considerable amount of asymptomatic carriers [17]. Thus, it is reasonable to assume infection data as underrepresented, with some proposals reaching 86% of false negatives [18].

Instead, mortality provides more reliable information due to its conclusive nature. However, mortality is not free from bias regarding COVID-19 [19] but seems comparatively less biased than infection. There is also some debate on the methodology to associate deaths to the disease in different countries but, if there is no accountability method change during the outbreak, the causal link from infection to occasional death translates in a reasonably constant scale factor.

The following section (Section 2) presents the mathematical model based on a differential equation that links the shape of the mortality curve to the disease duplication time, the time to develop immunity and the fraction of infected people. It seems important to highlight that these links are extracted from the curve shape and not from its magnitude, especially the one regarding the fraction of infected people. All this provides information on the number of infected people, even when the lethality of the disease is unknown, and before an outbreak has concluded. Section 3 applies the model to the Madrid and Andalusia COVID-19 cases. Section 4 further discusses the results and evaluates the suitability of government decisions. Conclusions close the work, issuing some practical recommendations.

2. A basic model for the evolution of the number of infections and its link to the mortality curve shape.

The proposed method is simple and based on the minimal number of parameters required for a reasonable spread description. Nevertheless, Section 3 confirms its explanatory and predictive power. The model has been presented in [24]. A brief explanation of the different terms in the proposed differential equation follows:

i) A first term is the number of infected individuals with the capability to transmit the disease. It is modeled by subtracting to the number of infected people at a given time, $N_i(t)$, the number of people that were already infected earlier than a particular time, t_{im}. The result is: $N_i(t) - N_i(t - t_{im})$ indicating that those who were infected before $t - t_{im}$, thanks to their immune system, do no longer infect other people.

ii) A second parameter is the fraction of people that are subject to be infected at a given time. It corresponds to the ratio between the non-infected people up to date, $N_{tot} - N_i$, and the total population N_{tot}, resulting in $(N_{tot} - N_i)/N_{tot}$. This value diminishes as transmitting individuals become surrounded by already infected and eventually immune individuals.
iii) These two parameters are connected by the average speed of transmission to non-infected individuals k.

Multiplying these terms, Eq. (1) defines the infected individuals' differential increase, $\mathrm{d}N_i$, during a differential time, $\mathrm{d}t$:

$$[N_i(t) - N_i(t - t_{im})] \cdot k \frac{N_{tot} - N_i}{N_{tot}} \cdot \mathrm{d}t = \mathrm{d}N_i \qquad (1)$$

The evolution is dependent only on three parameters: t_{im}, k and N_{tot}. For constant values in these three parameters the equation can be integrated yielding:

$$N_i = N_{tot} \cdot f_f \frac{2^{f_f(t-t_p)/t_d}}{1+2^{f_f(t-t_p)/t_d}}; \qquad \text{where } t_d = \frac{\mathrm{Log}_n(2)}{k} \text{ and } \left(1 - f_f\right)^{1/f_f} = 2^{-t_{im}/t_d} \qquad (2)$$

where Log_n refers to the Napierian logarithm based on the Euler number e. Parameters k and t_{im} have been exchanged for t_d and f_f because they have a physical meaning closer to the spread dynamics. The additional parameter, t_p, is the integration constant. Its value corresponds to the location in time of the maximum daily increment of infected individuals. It indicates if the outbreak has started sooner or later. The equation for the daily new infected cases is easily obtained from Eq. (2) yielding:

$$\Delta N_i = \frac{\mathrm{d}N_i}{\mathrm{d}t}\Delta \mathrm{t} = N_{tot} \cdot f_f^2 \frac{\mathrm{Log}_n(2)}{t_d} \frac{2^{f_f(t-t_p)/t_d}}{1+2^{f_f(t-t_p)/t_d}} \left(1 - \frac{2^{f_f(t-t_p)/t_d}}{1+2^{f_f(t-t_p)/t_d}}\right) \Delta t \qquad (3)$$

In Eq. (3) Δt accounts for the time of a day in the current time units. Figure 1 represents the curves, familiar to disease spreads, given by Eq. (2) and (3). It can be observed that f_f is the final fraction of the total population that is infected before the disease subsides, just for the case of no lockdown or any other containment ban. t_d is the disease duplication time in the absence of immunity ($f_f \longrightarrow 1$) and without limitations on the population ($N_{tot} \longrightarrow \infty$).

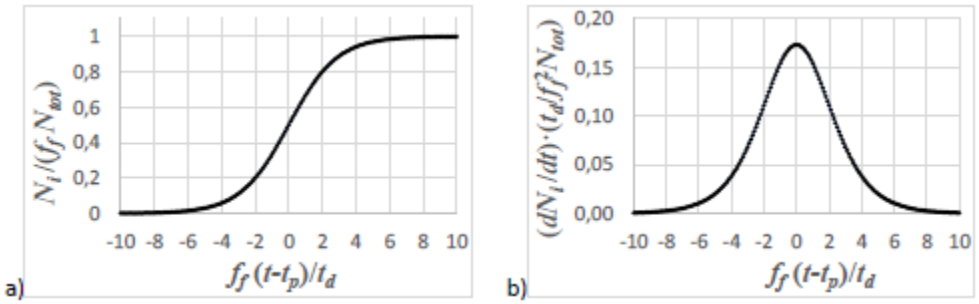

Figure 1: Disease with immunity development, without contaiment: a) Evolution of the number of infected persons, N_i, and b) Daily increment of such number, $\Delta N_i/\Delta \mathrm{t} = \mathrm{d}N_i/\mathrm{d}t$. The f_f factor indicates that not all the population gets infected. It also reduces the speed of the time evolution of the outbreak.

In order to obtain the four parameters of the model (t_d, f_f, t_p, and N_{tot}), the data of infected people seems more questionable than the mortality curve. Thus, the fourth step is to establish the link between the infected and mortality curves. This work considers $N_{fat}(t) = IFR \cdot N_i\left(t - t_{fat}\right)$, modeling the mortality curve by scaling and adding a delay time to the infection curve. In this model, IFR and t_{fat} are respectively, the infection fatality rate and the average time-lapse from infection to eventual death outcomes. Eq. (4) indicates the shape of the mortality curve for constant values of the commented parameters. For simplicity, t_{pfat} has been written instead of $t_p + t_{fat}$ for the time location of the peak of the mortality curve.

$$N_{fat}(t) = IFR \cdot N_i(t - t_{fat}) = IFR \cdot N_{tot} \cdot f_f \frac{2^{f_f(t-t_{pfat})/t_d}}{1+2^{f_f(t-t_{pfat})/t_d}} \quad (4)$$

The close resemblance between curves given in Eq. (2) and (4) is questionable, given that different patients would evolve at a different pace. The effect is a gaussian blurring of the curve. Nevertheless, this is considered in the Discussion section, indicating that f_f would be larger than the ones obtained and that the obtained numbers are conservative for the evaluated cases.

If there is a change in the value of the commented parameters, Eq. (1) cannot be integrated. In this case, to fit the mortality curve, Eq. (5) can be used instead of Eq. (4). This differential equation is obtained from Eq. (1) by scaling it with the IFR factor.

$$\left[N_{fat}(t) - N_{fat}(t - t_{im})\right] \cdot k \frac{IFR \cdot N_{tot} - N_i}{IFR \cdot N_{tot}} \cdot \mathrm{d}t = \mathrm{d}N_{fat} \quad (5)$$

In the following section, Eqs. (4) and (5) are used to evaluate the virus spread dynamics in Madrid and Andalusia, obtaining very different results.

3. Model fitting to the cases of Madrid and Andalusia

3.1 Madrid Community (Spain).

The Madrid Community mortality curve data has been made publicly available by the Spanish government. Large black dots in Fig. 2 depict the daily and accumulated mortality curves up to May the 25th. It is remarkably noisy data. Nevertheless, previous fittings of clearer cases processed by the authors, like Lombardy in Italy [24], support the fitting procedure. The amount of noise is mainly due to two facts:

(i) There is no data available for March the 8th and 9th. The same value is reported for cumulative mortality on March the 15th and the 16th (while increments of 127 and 142 deaths were reported on the previous and following days). Thus, only data after these dates have been used for the fittings below.

(ii) The lockdown was not made in a single step but two close phases. First, the local government suspended all educational activity on March the 11th; then, the national government dictated the lockdown on the 14th.

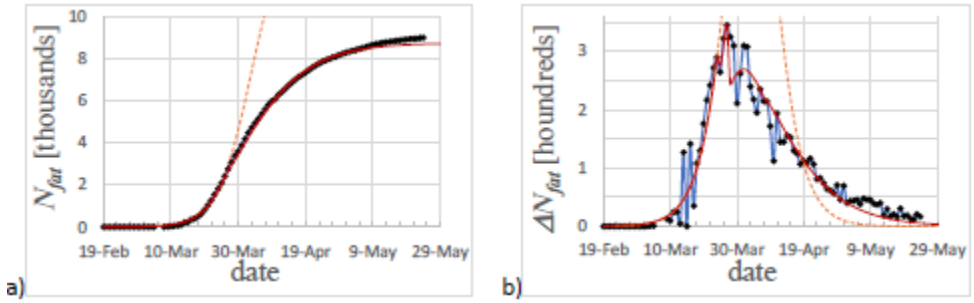

Figure 2: Madrid Covid-19 case mortality curves. Black dots indicate actual data. The continuous red line indicates the data fit up to 9/05/2020. The orange dashed corresponds to the estimated evolution without lockdown (it can be better traced in Fig. 4). a) Evolution of the number of fatalities, N_{fat}, and b) Daily increment of such number, ΔN_{fat}.

In reference [24] the authors observed a 14 days delay between the infection curve and the mortality curve. This is coherent with the approximate evolution of the disease (still under debate): 5 days from infection to first symptoms + 7 days of evolution with mild symptoms + 7 days of intense symptoms. The lockdown effect is evident in the mortality curve from March the 28th, displaying this 14 days delay. Also, the footprint of the suspension of the educational activity is evident from March 25th, exhibiting the same delay. Due to these effects, the fitting for this data has been split into three intervals:

(i) Up to March the 24th, the line is fitted with a curve that follows Eq. (4). In this equation, there are three parameters to fit: $(IFR \cdot N_{tot} \cdot f_f)$, (f_f/t_d) and (t_{pfat}). The brackets are included to highlight that the shape of the curve does not allow to discriminate individual parameters inside each group. This interval is a small portion of the outbreak behavior in absence of containment measures (orange dashed line in Figures 3 and 4). The fitting is performed imposing the value of the daily increment corresponding to the 24th and fitting the accumulated mortality curve by minimizing the RMS error. The parameter associated with the spread velocity of the disease, (f_f/t_d) = 0.29, is obtained with reasonable accuracy. But for the other two parameters the fitting is satisfied by any value following the relation $(IFR \cdot N_{tot} \cdot f_f)/1992 = 1{,}226^{(t_{pfat})}$ where N_{tot} is measured in persons and t_{pfat} is measured in days after the 24th and longer than 7 days. This is so because the denominator in Eq. (4), $1 + 2^{f_f(t-t_{pfat})/t_d}$, is close to 1 for the whole interval. Thus, they cannot be individually discriminated without information from the rest of the intervals.

(ii) From March the 25th up to the 27th, the change of the spread parameters imply that the equation cannot be integrated. Thus, Eq. (5) has to be used instead of (4). This equation requires the previous history as input. So, the function from the previous paragraph is used as bootstrapping. The parameters to fit into this equation are: $(IFR \cdot N_{tot})$, (k) and (t_{im}). The three days interval is too short to provide the 3 values and only (k) = 0.196 days^{-1} can be obtained. The other two parameters are obtained in the following paragraph. The fitting is reached imposing the daily increment corresponding to the 27th.

(iii) From March the 28th up to May the 9th, there is the period corresponding to the lockdown, counting with the 14 days delay from any action to its effect on the mortality curve. As in the preceding paragraph, Eq. (5) has to be used. Distinctly, this period is large enough to fit the three parameters. This is done iteratively, as the result is used to complement the value of the missing parameters in the previous two intervals. The values obtained are $(IFR \cdot N_{tot})$ = 16 500, (k) = 0.128 days^{-1} and (t_{im}) = 10 days. The fitting of t_{im} is done by imposing the location of the local maximum around April the 1st. The sudden change in the mortality curve slope around March the 27th due to the lockdown, produces this maximum, allowing for a suitable fitting of t_{im}. With this constraint, the rest of values are fitted by minimizing the RMS error. The amplitude of the second peak in the figure indicates that a better fit could be obtained by weighting the infection capability as a function of the time after infection. But this would unnecessarily increase the complexity of the model for the objective pursued in this paper.

The red line in Fig. 2 plots this fitting. Figure 2b) shows that the data on March the 22nd, 14 days after March the 8th, has some upwards deviation. It coincides with the celebration of the International Women's Day on March the 8th, gathering 120 000 people only in Madrid city center. It is apparent that the amount of deviation is within the rest of the noise, not impairing the use of the tool. Table 1 summarises the results of the fit together with the Andalusia case.

The curve fitting provides some relevant values regarding the outbreak dynamics. The most relevant is the one corresponding to the IFR. To obtain it, it has to be considered that the effect of the lockdown is two folds: (i) It reduces the spread velocity by reducing the frequency of contacts between persons. (ii) It may create groups of disease-free persons that interact with the rest of the population little enough to keep their group disease-free. This last effect would reduce the effective N_{tot} during lockdown. Thus, the effective N_{tot} would be any number smaller than the total Madrid population of resulting in $N_{tot,\,max}$ = 6.7 million. This implies that the minimum infection fatality rate would be $IFR_{min} = 0.0025$.

Antibodies-blind tests are another way to try to obtain the percentage of people that have not had any contact with the virus. These tests are currently underway. The preliminary results in Spain, [25], indicate that around 87% of the people with positive PCR test, develop a positive antibodies test response about 24 days after the symptoms. It also establishes that the ratio between positive antibody tests and fatalities is around 0.01. This would imply a corresponding $IFR_{max} = 0.0087$ in coincidence with other reports in USA, [26]. Locally, study [25] seems to have relevant flaws in the statistics, probably in the selection of population, generating a relevant deviation with respect to stroke incidence. In particular, it assesses 6 times more mortality with respect to antibody test positive response in La Rioja Community (Spain) than in Andalusia Community. Ethnicity, sanitary system and population pyramid are too similar to explain this discrepancy. Thus, only the global value for all Spain has been considered. This result has been tagged as maximum IFR because it does not take into account effects like the cross-immunity. Some reports on cross-immunity for Covid-19 indicate that as much as 40 to 60% of the population may have immune system responses to this virus as a result of previous exposition to a similar endemic mild virus, like HCoV-OC43 and HCoVNL63 [27]. A dedicated study of family in close contact with asymtomatics may improve the conclusions of [25].

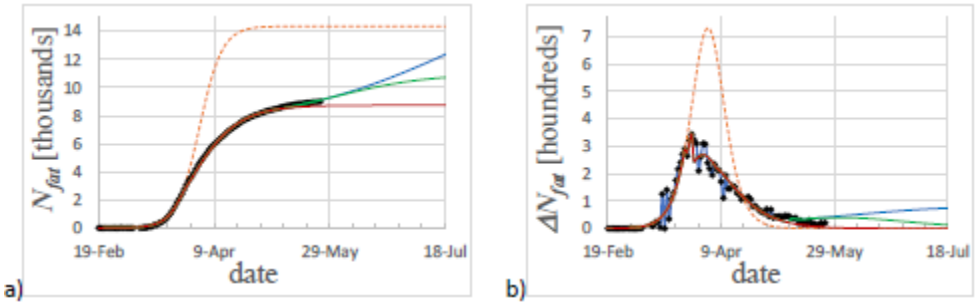

Figure 3: Effect after the 9/05/2020 of lifting containment measures in Madrid the 26/04/2020 (the blue and green continuous lines are commented in the text below). Same codes as in Fig. 2 for the rest of symbols. a) Evolution of the number of deaths, N_{fat}, and b) Daily increment of such number, ΔN_{fat}.

With the previous consideration and the parameters in Table 1, it is possible to evaluate the consequences of lockdown lifts. The Spanish government has proclaimed a relief for the lockdown on April the 26th by allowing children to go out on the streets with parental control. Also, a gradual lockdown lifting starting on

May the 4th is taking place in Spain (in Madrid it is delayed to start it on May the 25th). Fig. 3 depicts the possible consequences of these measures. The behavior of the outbreak after April the 26th can be observed in the mortality curve evolution after May the 9th, with the 14 days delay already commented. In this respect:

- The green continuous line in Figure 3, indicates the predicted behavior considering IFR = 0.0025 in combination with the largest spread velocity (corresponding to the scenario before the lockdown). This is the worst scenario for IFR = 0.0025.
- The blue continuous line in Figure 3, indicates the predicted behavior considering IFR = 0.0087 in combination with the smallest spread velocity (corresponding to the scenario during the lockdown). This is the best scenario for IFR = 0.0087 if the relief measures restore the population connectivity.

If the mortality curve evolves below the blue line, it indicates that either IFR = 0.0087 is not possible or that a relevant part of the population is still isolated away from contamination. If the mortality curve evolves above the green line, it indicates that IFR is larger than 0.0025.
Currently, the evolution is below the green line, but it is plausible that the connectivity in the population has not changed excessively. On June the 8th, both lines should be recalculated to check for the initial part of the containment lift. Nevertheless, it can be observed that, for Madrid case, it is easy to observe alarm signals that would allow the authorities to take containment measures on time.

3.2 Andalusia Community (Spain).

Lifting the lockdown in Madrid shows a moderate effect on the mortality curve. This is attributable to the presence of a large number of immune people in its population. Thus, it is relevant to evaluate the same effect on other populations. Focussing on Spain, Andalusia is one of the regions where the outbreak strike has been lighter. Thus, it constitutes an ideal second case to evaluate. Figure 4 depicts the daily and accumulated mortality curves. Benefitting from the Madrid case analysis, the values of t_{im} and IFR can be fixed, given the close ethnicity and age distribution of the population. Table 1 shows the result of the best fit for the rest of parameters. The duplication time is reasonably close to the Madrid case. Thus, the smaller number of deaths is due to a significant time delay concerning the local beginning of the disease outbreak. This delay corresponds to the two weeks of time difference between the peaks of the orange dashed lines in Figures 3 and 5. Although the applied mathematical model is the same as for the previous case, distinct conclusions arise. In this case, there was no suspension of the educational activity before the lockdown. Thus, the fitting procedure is split only in two intervals. One previous to March the 28th and the other from that date up to May the 9th. In both intervals, the fitting has been done by minimizing the RMS error. Figure 4 shows the mortality curves together with the best fit.

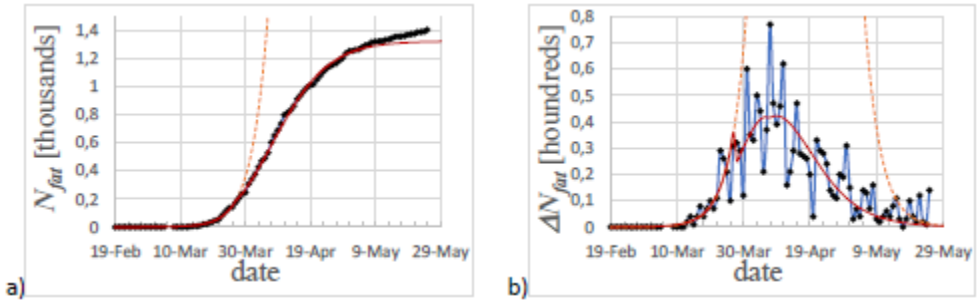

Figure 4: Mortality curves for the Andalusia Covid-19 case. Same symbol code as Fig. 2. a) Evolution of the number deceases, N_{fat}, and b) Daily increment of such number, ΔN_{fat}.

Although the data is noisy, the small number of parameters for the fit allows for a robust assessment of the parameters. During the lockdown, the value of $IFR \cdot N_{tot}$ = 1951 is obtained. The Andalusia population is 8.5 million people. If all the population was involved in the outbreak, the fitted value would imply an IFR as low as 0.0002. This value is ten times smaller than for the Madrid case. The close ethnicity and sanitary contradicts this possibility. A much more plausible theory is that the low population density allows for the formation of relevant isolated sectors with and without disease outbreak. Taking this into account and considering an IFR close to the one of Madrid (IFR = 0.0025), the total amount of the population subject of being infected during the considered dates is 0.8 million persons. In this situation, the lift of the lockdown generates a more complicated and hazardous situation than the Madrid case. Even if the lift is progressive and starts with timid measures (e.g., the opening of some services like hairdressing), the resulting social contact could generate connectivity between the commented sectors.

As in the Madrid case, the mathematical model allows evaluating the consequences of lockdown lifts. Fig. 5 depicts the possible consequences of relief measures.

Like in the Madrid case, the 14 days delay projects the footprint of the outbreak after April the 26th over the mortality curve after May the 9th. In this respect:

- The green continuous line in Fig. 5 indicates the predicted behavior considering IFR = 0.0025 in combination with the largest spread velocity (corresponding to the scenario before the lockdown). This is the worst scenario for IFR = 0.0025.
- The blue continuous line in Figure 5, indicates the predicted behavior considering IFR = 0.0087 in combination with the smallest spread velocity. In this case, the Madrid spread velocity during the lockdown has been chosen. It corresponds to a smaller velocity than the one of the Andalusia case. This choice avoids effects that could correspond to the strong lack of connectivity in Andalusia during the lockdown. This is the best scenario for IFR = 0.0087 if the relief measures restore the connectivity of the population.
- The grey continuous line in Fig. 5, indicates the predicted behavior considering IFR = 0.0025 in combination with the smallest spread velocity (again the Madrid spread velocity during the lockdown). This is the best scenario for IFR = 0.0025 if the relief measures restore the connectivity of the population to the level of connectivity in Madrid during the lockdown.

The mortality curve between the May the 10th and May the 17th, with 4.75 average daily fatalities, is below the three lines indicated above. Average daily fatalities of 19.2, 7.4, and 6.9 for green, blue, and grey curves, respectively. This indicates that the connectivity in the population has not changed excessively with the relief of children going out on the streets. From May the 18th, the three lines should be recalculated to check for the initial part of the containment lift. Nevertheless, it can be observed that, for the Andalusia case, the risk of a rebound is much larger than for the Madrid case.

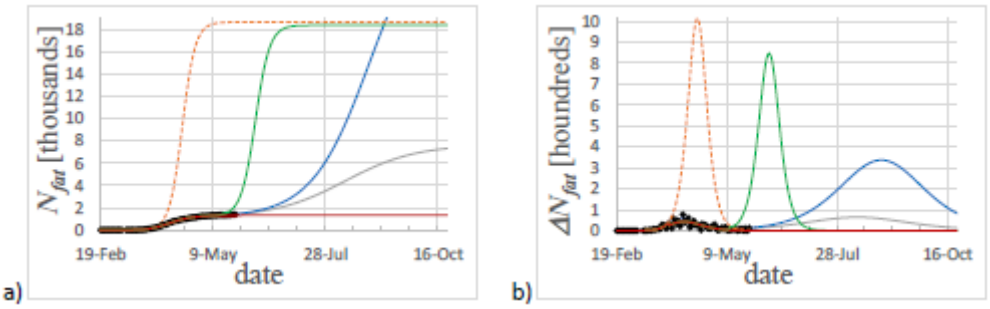

Figure 5: Effect of lifting containment measures in Andalusia from 26/04/2020 (the blue, green, and grey continuous lines are commented in the text below). Same codes as in Fig. 2 for the rest of the symbols. a) Evolution of the number of deaths, N_{fat}, and b) Daily increment of such number, ΔN_{fat}.

Table 1: Results of the fits on the Madrid and Andalusia mortality curves up to May the 9th (Outbreak behavior up to April the 26th), considering IFR = 0.0025.

		Madrid fit	Andalusia fit
Fitted parameters	t_{im}	10 [days]	10 [days]
	f_f	0.87	0.89
	IFR	0.0025	0.0025
	t_d (before lockdown)	3.0 [days]	2.8 [days]
	t_d (suspension of educ. activ.)	3.6 [days]	--------
	t_d (after lockdown)	5.4 [days]	4.3 [days]
	N_{tot} (non-isolated population after lockdown)	6.7 million pers.	0.8 million pers.
Main conclusions	Local population	6.7 million pers.	8.4 million pers.
	Infected people, N_i, on March the 14th (related to mortality curve on March the 28th)	1.2 million persons	0.1 million persons
	Infected people, N_i, on April the 26th (related to mortality curve on May the 10th)	3.5 million persons	0.5 million persons
	Deaths, N_{fat}, if lockdown is maintained indefinitely	8754 persons	1315 persons
	Deaths, N_{fat}, doing a lockdown lift on April the 26th without sanitary measures (green line).	11 034 persons	18 364 persons

Note: It should be noted that $t_d = \mathrm{Log}_n(2)/k$ is a reference duplication time. To yield the effective duplication time, it is modulated in Eq. (1) by the percentage of the infected population and the number of immune people.

4. Discussion and recommendations

The analyzed data indicates a significant difference in future predictions and hazards from zones strongly hit by the pandemic and those with less impact. Tools like the one presented are relevant for decision-makers. The first step is to learn from the past effects on the pandemic of already adopted measures. The global efficiency of lockdowns is a clear issue to analyze. Considering the case of Madrid and assuming an IFR = 0.0025, a complete lift of the lockdown by April the 26th would lead to a final count of 11 034 deaths. The absence of lockdown would have led to 14 400 deaths (if the sanitary system would have not collapsed in such a situation). This predicts that the lockdown, together with suspension of the educational activity has saved 3.4 thousand lives so far. A larger IFR would mean fewer lives saved with the lockdown. In particular, IFR = 0.0087 would reduce the number of saved lives to 2.7 thousand.

The counterpart is a profound impact on the economy. The link between GDP (Gross Domestic Product) and life expectancy is generally accepted [22]. In general, larger GDP per capita leads to larger government investment in the health system, and it increases the life expectancy of the population. Adding together the life expectancy increment for each person and dividing it in 30 years packets, it can be established that GDP in a community like Madrid saves between 300 and 900 lives a day (i.e. between 12 and 38 thousand lives along the 42 days of lockdown). This is a number more significant than the one associated with the direct lockdown effect on Covid-19 patients, which prevented the corresponding GDP. This results in an effective loss of lives. Nevertheless, the relevance of the lockdown lies not only in the number of lives saved but also on preventing the sanitary system from a collapse that would have generated many collateral additional deaths and psychological and economic effects.

The warning signal appears when the same analysis is applied to the Andalusia case. A complete lifting of the lockdown by April the 26th would lead to a final count of 18 364 deaths. This is considering the best case of complete lift without sanitary measures (green line) that includes using the virus spread velocity of Madrid without lockdown, smaller than that of Andalusia. The absence of lockdown would have led to 18 643 deaths. This predicts that the lockdown has saved 0.3 thousand lives so far. In the meantime, each day of Andalusia GDP saves the equivalent to 200 to 300 lives. Figure 6 indicates the directly Covid-19 daily saved lives in Madrid and Andalusia with the commented measures.

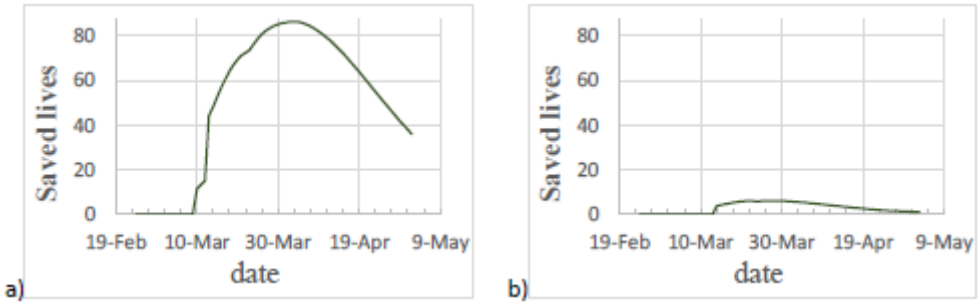

Figure 6: Daily saved lives during the lockdown + suspension of educational activity. a) Madrid case, total account = 3.4 thousand lives. b) Andalusia case, total account = 0.7 thousand lives.

Although the lockdown in Andalusia does not seem to have been a good idea, decision-makers had no information on the disease mortality or the spread dynamics before the outbreak arises. Now that society has the information, it should be used for future management.

A completely different perception of the lockdown arises if the virus is effectively eradicated from Andalusia with future strategies of location and isolation of infected people in the period in which they transmit the disease. Also, it would be different if the virus has a seasonal behavior and vanishes in summer or a vaccine is obtained. In all these cases, the delay on the spread thanks to the lockdown may result in a favorable life-saving strategy. This makes monitoring and double-checking variations of the spread parameters one of the main labors for the government.

An additional issue that complicates the scenario is the possibility of the formation of isolated groups carrying the disease during the lockdown, while the rest of the population does not develop any immunity. It represents a hazard of sudden expansion if reconnected to the general population as commented in Section 3 for Andalusia. This can probably be related to the low population density in Andalusia (less than 100 inhabitants/km^2) in comparison with communities like Madrid (around 800 inhabitants/km^2).

Based on this complex scenario, this study suggests the possibility of separated age strategies to reduce the pandemic impact. It makes sense if the detection and isolation of each person in the disease-transmitting period are not possible. The Spanish Lethality data [23] indicates that out of 216 848 tracked cases, the lethality is 25 times larger for people older than 50 years than for younger ones. Also, the number of cases for the first group is more than twice the cases of the second group. Given this large differences, for an IFR =

0.0025 and considering the Spanish population pyramid (41,2% of the population at older than 50), the resulting IFR for 50 and older is IFR_{50+} = 0.0061. Below that age, IFR_{49-} = 0.0001. This means that the outbreak is less hazardous for young people than driving their cars. It would be reasonable to let them make the decision on being lockdown or not. With the correct management, those deciding to make a normal life would generate an immune people layer protecting the elder. At the same time, de GDP would be fairly maintained. If the lockdown measures are lifted, taking this into account would mean a win-win strategy.

COVID-19 is still spreading across the globe; thus, this model has the potential to prevent adverse impacts in countries' disease developments. More concretely, it can be applied country and region-wise, and extract recommendations for lockdown liftings. Thus, under the light of this study, the governments should consider lockdown lifting to be region-wise and make predictions and monitoring based on this and other models. In fact, the conclusions indicate there is enough data to consider that starting to lift the lockdown on May the 4th at Andalusia while delaying it at Madrid is not the most correct procedure. Also, the beginning of this Section establishes that lockdowns may not be an optimal saving lives strategy. Thus, age-wise strategies should be strongly emphasized by governments. Very especially the care for not taking the virus home to our elders. This seems to be general knowledge, but very under-publicized in general.

Additionally, eventually expanded, this model seems especially appropriate for developing countries in which COVID-19 is still at an early stage, and where their governments can minimize impacts on the economy while maximizing healthcare and mortality prevention. Future studies to test the model with new data and the use of blind antigen, antibody, and cross-immunity responses testing to double-check critical parameters, are encouraged.

However, the model has limitations. Since COVID-19 data is still under development, unexpected behaviors can arise from third variables (e.g., virus mutations). Besides, the amount of time to develop symptoms makes difficult the assessments and can lead to significant underrepresentation of infection [18].

There has been debate about the accountability of deaths attributable to the COVID-19 virus. Including not tested patients, the number might increase by roughly 39% [28]. This would mean a death count underestimation by 39% in the results.

6. Conclusions

This study proposes and tests a model for providing infection parameters from mortality curves in rapid disease outbreaks. The feasibility of the model has been tested for Covid-19 outbreaks at Madrid and Andalusia in Spain. The average delay between infection and death occurrences is t_{fat}= 14 days. The average period from the moment an individual can infect, to the moment in which his immune system removes this possibility is t_{im}= 10 days. The infection-fatality rate lower limit is IFR_{min} = 0.0025. Basic disease duplication time in the absence of containment measures is close to 3 days. Basic disease duplication times during lockdowns is close to 4.8 days. The effective virus spread velocity depends on these times, in combination with the fraction of infected population and period of active disease transmission for an infected person.

The model can generate predictions for lockdown lift for the selected locations. Regarding Madrid, the model suggests a small increase in mortality that can be lessened with sanitary measures and is assumable for healthcare resources. However, the model predictions concerning a rebound for Andalusia, with increased mortality, should be considered as a warning signal and the management of the disease must be carefully planned. The results herewith encourage age-based strategies for such management. The presence of isolated groups of the population, respectively free and contaminated, with the disease can be diagnosed by the model helping in the development of contention strategies. The analysis indicates that some government decisions when the information was not available may be far from idoneus. This includes the lockdown in Andalusia, the delay in starting lockdown lifting in Madrid, the insufficient publicity to age-based sharp differences, and the protection of elders. The tool is inexpensive and affordable for any government and needs only reasonable skills to obtain forecasts.

7. Acknowledgments

The partial funding by project (UC3M-2009/00415/002) and support by "Instituto Universitario de Desarrollo Tecnológico y Promoción de la Innovación "Pedro Juan de Lastanosa", at Universidad Carlos III de Madrid and and by Institute in Research applied to Aeronautic Industry (INAIA), at Universidad de Castilla La Mancha, is greatly appreciated.

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Monitoring Biodiversity & Restoring Marine Ecosystems

by Roberto Danovaro, Member EUAS

Short Biography

Roberto Danovaro was born in Genoa (degrees in 1988). PhD in Environmental Sciences at the University of Pisa in 1993. Full Professor in Marine Biology and Ecology from 2001 at the Polytechnic University of Marche. Director of the Department of Marine Sciences (2004 to 2010), Director of the Department of Life and Environmental Sciences (2011 to 2014) at the Polytechnic University of Marche. Pro-Rector (Delegated to the Research) at the Polytechnic University of Marche (2010-2013). President of the Scientific Council of WWF Italy, Steering Board Member of OECD (Fostering Innovation in Ocean Economy). Member of the Scientific Council of several research institutions and panels (IUCN, UNEP, EU), Editor in Chief of international journals and coordinator of several international and EU programs (Horizon2020, DG ENV, EASME). President of the Italian Society of Ecology (2011-2013), and of the Italian Society of Limnology and Oceanography (2008-2011). President of the European Federation of Scientific Technological Societies (2008-2012). Member of the EU Academy of Sciences. RD received several Awards, including the World Prize BMC Biology (London, 2010), the Award of French Society of Oceanography (2011), and the ENI Award "Protection of the Environment" (2013). Nominated in 2013 by the Italian Ministry of Education University and Research (MIUR), President of the Stazione Zoologica Anton Dohrn (National Institute of Marine Biology Ecology and Biotechnology). In the 2018 was renewed as President of the SZN (2018-2022). (RD Scientometric data: H index - 82; articles on ISI journals with IF >450; citations>23.000).

Selected Publications and their citations (Google Scholar®)

Ecological variables for developing a global deep-ocean monitoring and conservation strategy

R Danovaro, E Fanelli, J Aguzzi, D Billett, L Carugati, C Corinaldesi et al
Nature Ecology & Evolution 2020, 4(2), 181-192 (Cit: 5; IF: 12.54)

The deep sea (>200 m depth) encompasses >95% of the world's ocean volume and represents the largest and least explored biome on Earth (<0.0001% of ocean surface), yet is increasingly under threat from multiple direct and indirect anthropogenic pressures. Our ability to preserve both benthic and pelagic deep-sea ecosystems depends upon effective ecosystem-based management strategies and monitoring based on widely agreed deep-sea ecological variables. Here, we identify a set of deep-sea essential ecological variables among five scientific areas of the deep ocean: (1) biodiversity; (2) ecosystem functions; (3)

impacts and risk assessment; (4) climate change, adaptation and evolution; and (5) ecosystem conservation. Conducting an expert elicitation (1,155 deep-sea scientists consulted and 112 respondents), our analysis indicates a wide consensus amongst deep-sea experts that monitoring should prioritize large organisms (that is, macro- and megafauna) living in deep waters and in benthic habitats, whereas monitoring of ecosystem functioning should focus on trophic structure and biomass production. Habitat degradation and recovery rates are identified as crucial features for monitoring deep-sea ecosystem health, while global climate change will likely shift bathymetric distributions and cause local extinction in deep-sea species. Finally, deep-sea conservation efforts should focus primarily on vulnerable marine ecosystems and habitat-forming species. Deep-sea observation efforts that prioritize these variables will help to support the implementation of effective management strategies on a global scale.

A high biodiversity mitigates the impact of ocean acidification on hard-bottom ecosystems

E Rastelli, B Petani, C Corinaldesi, A Dell'Anno, M Lo Martire, C Cerrano & R Danovaro
Scientific Report 2020, 10:2948 (IF:3.998)

Biodiversity loss and climate change simultaneously threaten marine ecosystems, yet their interactions remain largely unknown. Ocean acidification severely affects a wide variety of marine organisms and recent studies have predicted major impacts at the pH conditions expected for 2100. However, despite the renowned interdependence between biodiversity and ecosystem functioning, the hypothesis that the species' response to ocean acidification could differ based on the biodiversity of the natural multispecies assemblages in which they live remains untested. Here, using experimentally controlled conditions, we investigated the impact of acidification on key habitat-forming organisms (including corals, sponges and macroalgae) and associated microbes in hard-bottom assemblages characterized by different biodiversity levels. Our results indicate that, at higher biodiversity, the impact of acidification on otherwise highly vulnerable key organisms can be reduced by 50 to >90%, depending on the species. Here we show that such a positive effect of a higher biodiversity can be associated with higher availability of food resources and healthy microbe-host associations, overall increasing host resistance to acidification, while contrasting harmful outbreaks of opportunistic microbes. Given the climate change scenarios predicted for the future, we conclude that biodiversity conservation of hard-bottom ecosystems is fundamental also for mitigating the impacts of ocean acidification.

Towards an Ecosystem-Based Marine Spatial Planning in the deep Mediterranean Sea

E Manea, S Bianchelli, E Fanelli, R Danovaro, E Gissi
Science of The Total Environment 2020, 715: 136884 (Cit: 1; IF: 6.55)

The deep sea covers about 79% of the Mediterranean basin, including habitats potentially able to deliver multiple ecosystem services and numerous resources of high economic value. Thus, the deep Mediterranean Sea represents an important frontier for marine resources exploitation, which is embedded within the European Blue Growth Strategy goals and agendas. The deep sea is crucial for the ecological functioning of the entire

basin. For this reason, the deep Mediterranean deserves protection from the potential cumulative impacts derived from existent and developing human activities. Marine Spatial Planning (MSP) has been identified as key instrument for spatially allocating maritime uses in the sea space avoiding spatial conflicts between activities, and between activities and the environment. Indeed, MSP incorporates the ecosystem-based approach (EB-MSP) to balance both socio-economic and environmental objectives, in line with the Maritime Spatial Planning Directive and the Marine Strategy Framework Directive. Despite MSP is under implementation in Europe, the Directive is not applied yet for the managing and monitoring of the environmental status of the deep sea. In the Mediterranean, deep areas fall both in internal and territorial waters, and in High Seas, and its management framework turns out to be complicated. Moreover, a certain level of cumulative impacts in the deep Mediterranean has been already identified and likely underestimated because of paucity of knowledge related with deep-sea ecosystems. Thus, the implementation of scientific knowledge and the establishment of a sustainable management regime of deep-sea resources and space are urgent. This study aims at reflecting on the best available ecological knowledge on the deep Mediterranean to incorporate conservation objectives in EB-MSP. We propose a framework to include key ecological principles in the relevant phases of any EB-MSP processes taking in consideration existing socio-economic and conservation scenarios in the region. We add the uncertainty principle to reflect on the still unexplored and missing knowledge related to the deep Mediterranean. Here, we resume some guidelines to overcome limits and bottlenecks while ensuring protection of deep-sea ecosystems and resources in the Mediterranean Sea.

Towards a marine strategy for the deep Mediterranean Sea: Analysis of current ecological status

R Danovaro, E Fanelli, M Canals, T Ciuffardi, M-C Fabrie, M Taviani et al
Marine Policy 2020, 112: 103781 (Cit: 8; IF:3.228)

The Marine Strategy Framework Directive (MSFD), introduced in June 2008, was adopted to achieve a Good Environmental Status (GES) in the EU's marine waters and to protect resources of socio-economic interest. The MSFD exerts to the marine area over which a Member State exercises jurisdictional rights in accordance with the United Nations Convention on the Law of the Sea (UNCLOS), including the deep-sea waters, seafloor and sub-seafloor of the Exclusive Economic Zones (EEZ). However, currently the MSFD focuses on coastal habitats and the shallow-water seafloor to the detriment of the deeper habitats. Despite the huge dimension of the deep sea (below 200 m of depth) covering more than 65% of the Earth's surface and including >95% of the global biosphere, the relevance of the dark portion of the seas and oceans is still almost completely neglected. Given the important bi-directional links between shallow and deep ecosystems, there is a clear need for extending the implementation of the MSFD into the deep sea, to define a sound ecosystem-based approach for the management and protection of deep-sea ecosystems and attain GES. We assembled data on drivers, anthropogenic pressures and impacts concerning the MSFD descriptors pertaining to the Mediterranean deep sea. We list deep-sea monitoring activities and the main sources providing benchmark conditions, and discuss knowledge and geographic coverage gaps. MSFD descriptors apply to the deep sea as to coastal waters, and ought to be monitored contemporaneously. We provide recommendations for guidelines for future deep-sea monitoring in the Mediterranean Sea.

A fast-moving target: achieving marine conservation goals under shifting climate and policies

G Rilov, R Danovaro, C Loiseau, J Claudet, S Katsanevakis
Ecological Applications, 30: e02009 (Cit: 8; IF: 4.248)

In the Anthropocene, marine ecosystems are rapidly shifting to new ecological states. Achieving effective conservation of marine biodiversity has become a fast-moving target because of both global climate change and continuous shifts in marine policies. How prepared are we to deal with this crisis? We examined EU Member States Programs of Measures designed for the implementation of EU marine environmental policies, as well as recent European Marine Spatial Plans, and discovered that climate change is rarely considered operationally. Further, our analysis revealed that monitoring programs in marine protected areas are often insufficient to clearly distinguish between impacts of local and global stressors. Finally, we suggest that while the novel global Blue Growth approach may jeopardize previous marine conservation efforts, it can also provide new conservation opportunities. Adaptive management is the way forward (e.g., preserving ecosystem functions in climate change hotspots, and identifying and targeting climate refugia areas for protection) using Marine Spatial Planning as a framework for action, especially given the push for Blue Growth.

Type 2 Topoisomerases and Prostate Cancer

by William Nelson, Member EUAS

Short Biography

Dr. Nelson serves as the Marion I. Knott Professor of Oncology and Director of the Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins. He completed undergraduate studies in Chemistry at Yale University, and earned doctoral degrees in Pharmacology and in Medicine at the Johns Hopkins University School of Medicine, Upon completing Internship and Residency training in Internal Medicine, Dr. Nelson undertook Fellowship training in Medical Oncology at the Johns Hopkins Hospital. After joining the Hopkins faculty, he rose through the ranks to Professor of Oncology, Medicine, Pharmacology, Pathology, Radiation Oncology, Urology, and Environmental Health Sciences.

Dr. Nelson's research has focused on cancer epigenetics and on prostate cancer development. He has now authored more than 290 journal article and book chapters, attracting >36,000 citations with an h-index of 100. He also has secured 11 issued patents from the US Patent and Trade Office, and has conducted some 67 podcast interviews. He currently serves on the Board and as Scientific Director of the V Foundation, as a Scientific Co-Chair for Stand Up 2 Cancer, and on the Scientific Advisory Board for the Prostate Cancer Foundation. He is also the Executive Editor of Cancer Today, a Senior Editor of Cancer Research, and on the Editorial Board of the Journal of Clinical Investigation.

Type 2 Topoisomerases and the Pathogenesis of Human Prostate Cancer

Type 2 topoisomerases are uniquely able to pass double-stranded DNA molecules through transient enzyme-catalyzed DNA double-strand DNA breaks [1]. Human cells contain two such enzymes, TOP2A and TOP2B; TOP2A acts preferentially in proliferating cells, preventing tangling of replicated DNA and promoting chromosome condensation to permit mitotic segregation, while TOP2B functions in interphase cells to facilitate regulated transcription [2-4]. In the healthy normal prostate, TOP2B is needed for activation of the androgen-regulated transcription program driving differentiation of columnar secretory cells [5]. TOP2B dysfunction in prostate cells appears responsible for *TMPRSS2-ERG1* gene fusions and other translocations characteristic of prostate cancers [4,5].

In the normal prostate, the androgenic hormone testosterone (T), and its 5α-reduced product dihydrotestosterone (DHT), bind to the androgen receptor (AR) in prostate cells, driving the receptor into the nucleus to bind to discrete androgen response elements (AREs) at the regulatory regions of genes like *KLK3* (encoding prostate-specific antigen or

PSA) and *TMPRSS2* involved in luminal cell differentiation [6]. In response to AR activation and genome engagement, the structure of chromatin in the cells undergoes marked reorganization for the purpose of reprogramming transcription, with looping of promoter and enhancer regions and the assembly of transcription hubs [7].

This chromatin transformation poses a significant challenge in DNA topology, risking tangling of DNA helices that can only be resolved by type 2 topoisomerases. In addition, transcription itself can create under-winding of DNA in the wake of advancing RNA polymerases and over-winding in front [8]. Also, RNA-DNA hybrid sequences forming R-loop structures can arise during transcription [9].

Not surprisingly, TOP2B was found to play a critical role in androgen-regulated gene expression [5]. When AR-expressing prostate cancer cells were starved of androgenic hormones and then exposed to DHT, the activated AR entered the cell nucleus and recruited TOP2B to AREs in regulatory regions of target genes. At these sites, TOP2B proved essential for the looping of promoter and enhancer sequences at genes like *TMPRSS2* into an active configuration ready to load RNA polymerase.

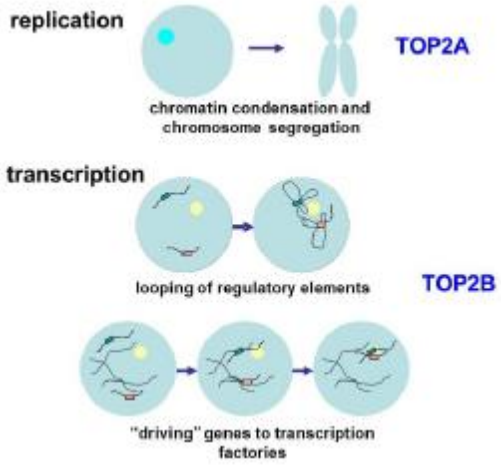

Figure 1. TOP2 Functions during replication and transcription.

II. Remarkably, TOP2B enzyme action was required for the initiation of the *entirety* of the AR transcription program in prostate cells.

Somatic fusions involving androgen-regulated genes, like *TMPRSS2*, and cancer genes, like *ERG1*, arise commonly in human prostate cancers [10].

With the insight that T and DHT could drive AR to recruit TOP2B to AREs in prostate cells, the possibility that TOP2B cleavage of double-strand DNA at these sites, required for passage of DNA helices during looping and untangling, might drive such translocations was explored. Ideally, TOP2-mediated double-strand cleavage comprises a short-lived event, sufficient for double-strand DNA passage. The cleavage reaction itself involves temporary covalent attachment of critical tyrosine amino acids in the enzyme to phosphodiester bonds at the broken DNA ends. When TOP2 is trapped in this reaction intermediate, such as upon exposure to drugs like etoposide, proteasome-mediated degradation of enzyme protein ensues, accompanied by removal of the remaining tyrosine residues covalently linked to the DNA ends by TDP2. The resulting DNA double-strand breaks are then repaired using non-homologous end-joining (NHEJ) [11-13]. In prostate cells grown in cell culture, TOP2B could be readily trapped by etoposide near ARE sites in *TMPRSS2* after androgen stimulation. These sites were congruent with mapped TMPRSS2

translocation sites mapped in prostate cancer cases [5,14].

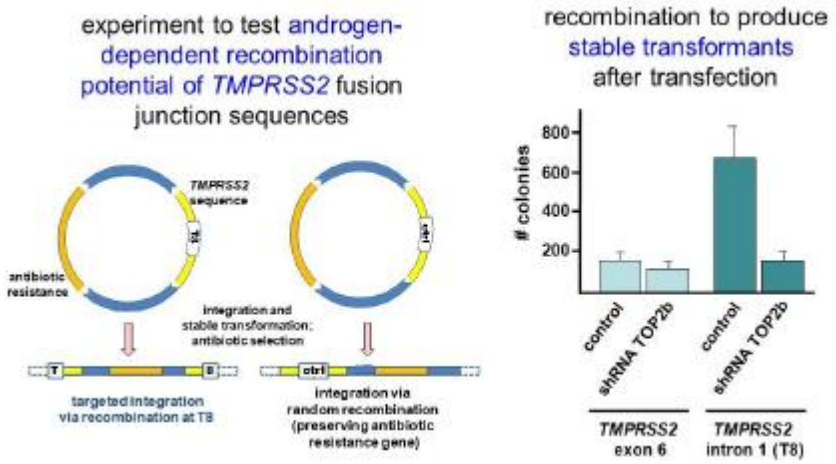

Figure 2. A sequence from TMPRSS2 intron mediates AR-and TOP2B-dependent recombination.

In a direct test of the hypothesis that TOP2B might be responsible for somatic translocations at AR target genes in prostate cancers, prostate cells stimulated with androgens created *TMPRSS2-ERG1* gene fusions *in vitro* in a manner requiring TOP2B [5]. Further evidence for AR-regulated TOP2B-mediated recombination was found when plasmid DNAs containing AREs along with selectable markers were driven to more efficient integration in prostate cells expressing AR, by virtue of TOP2B cleavage and NHEJ repair at ARE sites [5]. Transformation by these ARE-containing plasmids was suppressed in the absence of AR or TOP2B. The basic mechanism by which TOP2B-mediated cleavage leads to *TMPRSS2-ERG1* gene fusions likely has important implications for other somatic cancer genome alterations affecting other types of cancers [15].

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New Contributions in Biorefining

by Arthur Ragauskas, Member EUAS

Short Biography

Arthur Ragauskas held the first Fulbright Chair in Alternative Energy and is a Fellow of American Association for the Advancement of Science, the International Academy of Wood Science and TAPPI. In 2014, he assumed a Governor's Chair for Biorefining based in University of Tennessee's Department of Chemical and Biomolecular Engineering, with a complementary appointment in the UT Institute of Agriculture's Department of Forestry, Wildlife, and Fisheries and serves in the US Energy and Environmental Sciences Directorate, Biosciences Division, at ORNL. His research program is directed at understanding and exploiting innovative sustainable bioresources. This multifaceted program is targeted to develop new and improved applications for nature's premiere renewable biopolymers for biofuels, biopower, and bio-based materials and chemicals. His research program has been sponsored by NSF, USDA, DOE, GA Traditional Industry Program, a consortium of industry partners, and several fellowship programs which is summarized in 488 publications. His Fulbright sponsored activities at Chalmers University of Technology, Sweden were focused on the forest biorefinery and new biofuel conversion technologies for lignocellulosics. Currently, Dr. Ragauskas manages a research group of graduate students, postdoctoral research fellows, a research scientist, and visiting scientists. He is the recipient of the 2014 TAPPI Gunnar Nicholson Gold Medal Award, the ACS Affordable Green Chemistry award, 2017 AIChE Green Processing Award, 2017 Academia Distinguished Service Award, and his students and postdocs have won several awards, including the ACS graduate research award, ORNL UT-Battelle Award, and Supplementary Performance Award (ORNL).

Ragauskas is an Associate Editor for Biofuels, Bioproducts and Biorefining, Biofuels, BioEnergy Research, Industrial Biotechnology, Taiwan Journal of Forest Service, TAPPI J., Holzforschung, Journal of Biobased Materials and Bioenergy, Journal of Petroleum Technology and Alternative Fuels, The Open Biotechnology Journal, Current Biotechnology, and J. Wood Chemistry and Technology. He is an editorial board member of Sustainability and Journal of Chemical Technology and Biotechnology. Ragauskas has served on several advisory boards and review panels including: Austrian Science Fund, European Commission Research Directorate, National Science Academy, J. Paul Getty Trust, NSF, USDA, DOE, ARAP-E, NSERC, TAPPI Research Management Committee, Netherlands Organization for Scientific Research (NWO), Swedish Foundation for Strategic Research, Swedish VINN Excellence Center, Swedish Knowledge Foundation, VTT Technical Research Centre of Finland, ERA Chemistry, Swiss National Science Foundation, Finnish Academy of Science Norway Research Council, The Technology Foundation STW, Agence Nationale de la Recherche and Singapore Agency for Science, Technology and Research. Dr. Ragauskas has been an invited visiting professor at Universidade da Beira Interior, Portugal; Chalmers University of Technology, Sweden; Royal Institute of Technology/ STFi, Stockholm, Sweden; and Southeast University, China, and South China University of Technology, China.

Ragauskas Governor Chair Mission Statement

As an academician, Ragauskas' core belief is that a professor can only be as successful as the students he educates, mentors, and graduates. As such, Ragauskas' academic mission has been, and remains, the cornerstone of his career objectives. These career objectives include:

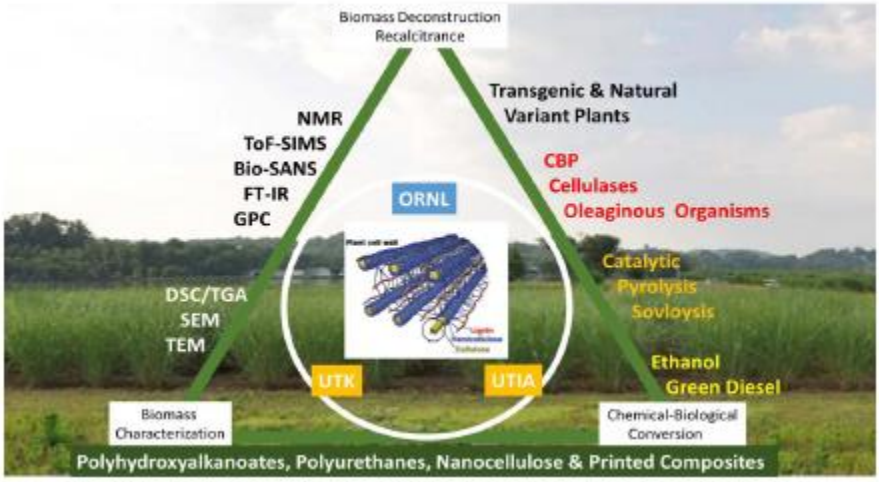
- Develop a challenging and enriching educational and research experience that facilitates the intellectual development of UTK/UTIA students and postdoctoral fellows and supports the mission of the Department of Chemical and Biomolecular Engineering, and Center for Renewable Carbon.

- Recruit, educate, and develop the next generation of scientists that will be nationally/internationally recognized leaders in green chemical engineering of biofuels, bio-derived materials, and chemicals.
- Develop a nationally/internationally recognized research center for sustainable green chemical engineering of biorefining, leveraging the exceptional researchers and research infrastructure located at ORNL, UTK, and UTIA.

Research Accomplishments and Activities

Ragauskas assumed the ORNL-UTK-UTIA Governor's Chair in Biorefining position in June 2014. This UTK faculty position, jointly funded by UTK/UTIA and ORNL, is focused on developing a fundamental research and academic program in sustainable biomass biorefining. As highlighted in Ragauskas' 2018 invited seminar at the Birmingham Science Museum (England), his research program is focused on three central overlapping focus areas (see **Figure 1**) including:

- Fundamental lignocellulosic properties of plant cell walls and their relationship to biological biorefining of biomass to biofuels.
- Valorization of biomass components for bio-derived materials
- Development of new tools and methodologies for biomass characterization.



F**ig. 1**. Summary of Ragauskas' ORNL, UTK, UTIA Governor Chair Research in Biorefining.

During this period, his research group has published over 200 manuscripts, of which greater than 90% were joint ORNL-UTK-UTIA publications. Of these publications, 59 publications were the outcome of research activities sponsored by BioEnergy Science Center (BESC, DOE-funded energy funded awarded to ORNL), 20 publications from ORNL's Center for Bioenergy Innovation (CBI, DOE funded) and 12 from ORNL's Science Focus Area "Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation." As such, Ragauskas' group remains the top publishing group from 2014 forward within BESC/CBI.

Ragauskas' publications are acknowledged internationally with a **Google H-index of 92**, **i10 inex of 395** and **greater than 36400 citations**. These overall accomplishments were awarded last year by Publons (Clarivate Analytics), who named Ragauskas as one of the world's most highly cited researchers in his field for 2018. The impact of these studies was recognized in a series of awards, including: 2019 AIChE Chase Award, Joint Faculty Award in Science and Technology, UT-Battelle (2019), Nominated to Sigma Xi (2019), Clarivate Analytics, Publons: Ragauskas named one of the world's most highly cited researchers in his field for 2018, FellowRoyal Society of Chemistry (2018), Green Process Engineering American Institute of Chemical Engineers Award (2017), University of California, Bourns College of Engineering – Center for Environmental Research and Technology, Distinguished Service Award (2017), TAPPI Gunnar Nicholson Gold

Medal Award (2014), ACS Award for Affordable Green Chemistry (2014), ORNL Visiting Fellow (2013), Elected American Association for the Advancement of Science Fellow (2012), Elected to Academy Board of International Academy of Wood Science (2012), Fulbright Distinguished Chair in Alternative Energy (2008-2009), Nominated to National Commission on Energy Policy (2008), Recipient of 2008 William H.Aiken Research Prize, Elected Fellow to International Academy of Wood Science (2003), Elected TAPPI Fellow (2003)

Representative Focused Activities: Five representative publications that have been published since Ragauskas assumed the Governor's Chair position include:

1. Downregulation of pectin biosynthesis gene GAUT4 leads to reduced ferulate and lignin-carbohydrate cross-linking in switchgrass. Li M.; Yoo C.G.; Pu Y.; Biswal A.K.; Tolbert A. K; Mohnen D.; Ragauskas A.J.; *Communications Biology* (2019) 2, 22.
2. Sugar release and growth of biofuel crops are improved by downregulation of pectin biosynthesis. Biswal, A.K.; Atmodjo, M.A.; Li, M.; Baxter, H.L.; Yoo, C.G.; Pu, Y.; Lee, Y.C.; Mazarei, M.; Black, I.M.; Ji-Yi, Z.; Ramanna, H.; Bray, A.L.; King, Z.R.; LaFayette, P.R.; Pattathil, S.; Donohoe, B.S.; Mohanty, S.S.; Ryno, D.;Yee, K.; Thompson, O.A.; Rodriguez Jr., M.; Dumitrache, A.; Natzke, J.; Winkeler, K.; Collins, C.; Yang, X.; Tan, L.; Sykes, R.W.; Gjersing, E.L.; Ziebell, A.; Turner, G.B.; Decker, S.R.; Hahn, M.G.; Davison, B.H.; Udvardi, M.K.; Mielenz, J.R.; Mark, D.F.; Nelson, R.A.; Parrott, W.A.; Ragauskas, A.J.; Stewart Jr., N.C.; Mohnen, D. *Nature Biotechnology* (2018) 36(3), 249-257.
3. Insights of biomass recalcitrance in *Populus* trichocarpa natural variants for biomass conversion. Yoo, C.G.; Yang, Y.; Pu, Y.; Meng, X.; Muchero, W.; Yee, K.; Thompson, O.; Rodriguez, M.; Bali, G.; Engle, N.L.; Lindquist, E.; Singan, V.; Schmutz, J.; DiFazio, S.; Tschaplinski, T.J.; Tuskas, G.; Chen, J.G.; Davison. B.H.; Ragauskas, A. *Green Chemistry* (2017) 19(22), 5467-5478.
4. A study of poplar organosolv lignin after melt rheology treatment as carbon fiber precursors. Sun, Q.; Khunsupat, R.; Akato, K.; Tao, J.; Labbe, N.; Gallego, N.C.; Bozell, J.J.; Rials, T.G.; Tuskan, G.A.; Tschaplinski, Timothy J.; Naskar, A.K.; Pu, Y.; Ragauskas, A.J. *Green Chemistry* (2016) 18(18), 5015-5024.
5. Cross-linked poly(methyl vinyl ether-co-maleic acid)/poly(ethylene glycol)/nanocellulosics foams via directional freezing. Liang, L.; Huang, C.; Hao, N.; Ragauskas, A.J. *Carbohydrate Polymers* (2019) 213, 346-351.

The first two publications, in the Nature family of publications, are representative of Ragauskas' collaborative efforts within BESC and CBI. In both of these publications, advanced analytical methodologies were employed to determine the structure and molecular properties of cellulose, hemicellulose, and lignin in the native and transgenic switchgrass samples grown by researchers at UTK and University of Georgia. These fundamental studies highlighted the unique role that lignin-carbohydrate complexes (LCC) contribute to reduced recalcitrance in the knockdown expression of GalactUronosylTransferase 4 (GAUT4) in switchgrass when compared to wild type (WT) switchgrass. The reduction in LCC linkages was hypothesized to facilitate lignin migration allowing for improved cellulase deconstruction after a hot water pretreatment (see **Figure 2**).

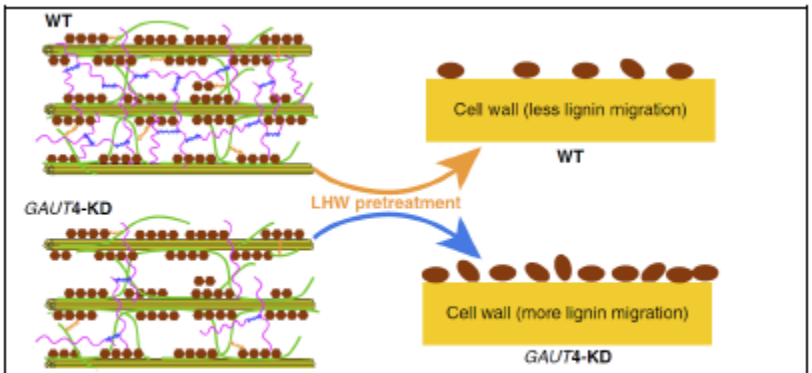


Figure 2. LCC impact on Wild Type and GAUT4-KD Switchgrass on Liquid Hot Water Pretreatment.

In light of the continuing controversies of LCC and methods of detecting these structures, Ragauskas was invited to submit a critical analytical review on this topic, along with research colleagues from the Royal Institute of Technology (Sweden), to Green Chemistry journal and this work was just recently published:

- A Critical Review on the Analysis of Lignin Carbohydrate Bonds in Plants. Giummarella, N.; Pu, Y.; Ragauskas, A.; Lawoko, M. *Green Chemistry* (2019) 20, 1573 - 1595.

The third publication is representative of Ragauskas' *Populus* research within BESC and CBI.

Working with a team of ORNL researchers, he has examined the sugar release performance of natural *Populus* variants and correlated their biomass recalcitrance properties to the fundamental structure of cellulose, hemicellulose, and lignin. Among the physicochemical properties of poplar, the lignin content, lignin molecular weight, lignin S/G ratio, and cellulose accessibility were found to strongly correlate with sugar release. The results demonstrated that the lignin content was negatively correlated with sugar release, whereas the lignin molecular weight, lignin S/G ratio, and cellulose accessibility were positively associated with poplar sugar release. These changes in biopolymer structures were then related by differential gene expression (DEG) to identify potential target gene groups that are correlated with recalcitrance factors (see **Figure 3**). These results provide valuable information for future biomass studies to understand the novel genes and their regulatory mechanism in forest genetics and apply this to tree breeding for enhancing biomass utilization.

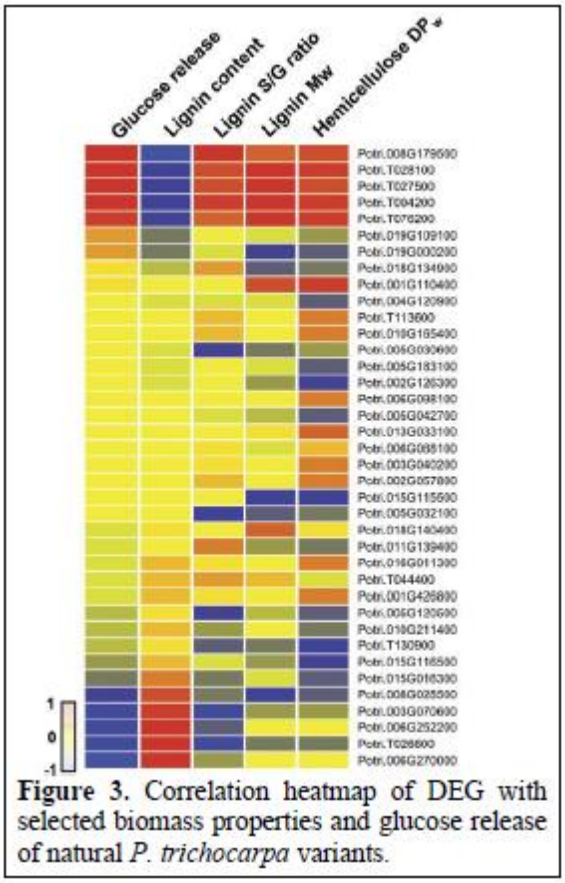


Figure 3. Correlation heatmap of DEG with selected biomass properties and glucose release of natural *P. trichocarpa* variants.

In all of these recalcitrance studies, lignin is a by-product that was historically viewed as either a waste product or, at best, a product for combustion. Starting with Ragauskas' publication in Science titled "Lignin Valorization: Improving Lignin Processing in the Biorefinery" (Ragauskas, A.J.; Beckham, G.T.; Biddy, M.J.; Chandra, R.; Chen, F.; Davis, M.F.; Davison, B.H.; Dixon, R.A.; Gilna, P.; Keller, M.; Langan, P.; Naskar, A.K.; Saddler, J.N.; Tschaplinski, T.J.; Tuskan,

G.A.; Wyman, C.E. Science, (2014) 344(6185), 1246843-1-1246843-10) he has focused on utilizing lignin as a feedstock for novel material applications. A key focus of these studies is to demonstrate that lignin structure is a critical factor in controlling physiochemical properties. This hypothesis was clearly illustrated in paper 4, whereby Ragauskas demonstrated viscosity properties of lignin at elevated temperatures could be altered by lignin's degree of polymerization and structural features. Comparable findings have also been reported in related studies, including:

- Linking lignin source with structural and electrochemical properties of lignin-derived carbon materials. Li, W.; Zhang, Y.; Das, L.; Wang, Y.; Li, M.; Wanninayake, N.; Pu, Y.; Kim, D.Y.; Cheng, Y.T.; Ragauskas, A.J.; Shi, J., RSC Advances (2018) 8(68), 38721-38732.
- Understanding lignin fractionation and characterization from engineered switchgrass treated by an aqueous ionic liquid. Liu, E.; Li, M.; Das, L.; Pu, Y.; Frazier, T.; Zhao, B.; Crocker, M.; Ragauskas, A.J.; Shi, J. ACS Sustainable Chemistry & Engineering (2018) 6(5), 6612-6623.
- Mechanism-Guided Design of Highly Efficient Protein Secretion and Lipid Conversion for Biomanufacturing and Biorefining. Xie, S.; Sun, S.; Lin, F.; Li, M.; Pu, Y.; Cheng, Y.; Xu, B.; Liu, Z.; Sousa, L.C.; Dale, B.E.; Ragauskas, A.J.; Dai, S.Y.; Yuan, J.S. Advanced Science, doi.org/10.1002/advs.201801980.

In addition to genetic factors controlling the structure of lignin in bioresources, the extraction of lignin from biomass and its impact on lignin structure has been clearly defined in a series of publications, including CBI studies working with researchers at University of California, Riverside. Examining the structure before and after CELF pretreatment, lignin structure was shown to exhibit a significant decrease in DP and an accompanying decrease in □-aryl ethers (Note: depending on CELF reaction conditions) as reported in:

- Hybrid Catalytic Biorefining of Hardwood Biomass to Methylated Furans and Depolymerized Technical Lignin. Seemala, B.; Meng, X.; Parikh, A.; Nagane, N.; Kumar, R.; Wyman, C.E.; Ragauskas, A.J.; Christopher, P.; Cai, C.M. ACS Sustainable Chemistry & Engineering (2018) 6(8), 10587-10594.

In contrast, the use of Consolidated Biomass Processing (CBP) yields residual lignin with minimally changes in structure, as reported in:

- Elucidating the structural changes to Populus lignin during consolidated bioprocessing with Clostridium thermocellum. Akinosho, H. O.; Yoo, C. G.; Dumitrache, A.; Natzke, J.; Muchero, W.; Brown, S.D.; Ragauskas, A.J., ACS Sustainable Chemistry & Engineering (2017) 5:9, 7486–7491.

Note: CBP is a biological deconstruction process which leads to conversion of plant polysaccharides to biofuel, while leaving behind the lignin.

The later finding is an important discovery since it allows future lignin valorization studies to be directly tied to the structural nature of lignin in plants. Currently, most pretreatments alter the structure of lignin, hence pretreatment lignin valorization studies need to consider both the structure of lignin in the starting biomass and the impact of pretreatment.

Concluding Statement

In summary, since the Governor's Chair position in the summer of 2014, Dr. Ragauskas' professional vision has been to leverage his past academic-research accomplishments in lignocellulosic chemistry to develop a nationally and internationally recognized program for fundamental sustainable green chemistry engineering of biorenewables for biofuels, bio-derived materials, and chemicals at ORNL, UTK, and UTIA.

Water Droplet Trajectories in an Irrigation Spray: the Classical and Quantum Mechanical Pictures

by Daniele De Wrachien, Member EUAS

Short Biography

Daniele De Wrachien is currently Retired Professor of Agricultural Hydraulics at the Department of Agricultural and Environmental Sciences of the State University of Milan and Member of the Board of Director of the Wessex Institute of Technology (WIT), Southampton, UK. He graduated from the State University of Milan as geologist and obtained his PhD in Advanced Engineering Geology. He performed his duties as ,Director of the Institute of Agricultural Hydraulics (2000-2006 ,Director of Computer Centre of the Faculty of Agriculture,(1992-95), Tutor of MPhil and PhD students of the Faculty of Agriculture External Examiner to MPhil and PhD students, Visiting Professor at the Wessex Institute of Technology (WIT). Daniele received the following Honours and Awards : Award for Truthful Support and Help in Organizing and Improving Scientific Level of the Symposia "Actual Tasks on Agricultural Engineering", Croatian Agricultural Engineering Society , Award in Recognition of Services to the European Society of Agricultural Engineers, Award for outstanding contribution to Engineering Sciences ,WIT ,Award for the Best Performing Working Body ,International Commission on Irrigation and Drainage.

Daniele is Author of over 150 scientific publications: papers, key-note lectures, books and technical reports and Member of the Editorial Board of the following International Journals :International Journal of Agricultural and Biological Engineering, 2009 : Journal of Agricultural Sciences (Editor-in-Chief) ,2010 , Journal of Irrigation&Drainage Systems Engineering (Executive Editor), 2010-,International Journal of Computational Methods and Experimental Measurements, 2010- ,Journal of Smart Grid and Renewable Energy, 2010 - Journal of Safety and Security Engineering ,2011- , International Journal of Advanced Renewable Energy Research , 2012-, American Journal of Experimental Agricultural (Editor-in-Chief) 2013 –, Journal on Frontiers in Soil Science , 2013- , Journal of Agricultural Science and Application,2013- ., Irrigation and Drainage (Associate Editor), 1998- .

Daniele has been involved in the organization of more than sixty International Conferences , Congresses, Symposia and Workshop in Africa ,America , Asia , Australia and Europe ,performing the role of Chairman, Key-note Speaker and Member of the Scientific and Organizing Committees.

As President of the European Society of Agricultural Engineers (2002- 04)Daniele established Agreements with national, regional and world-wide Organisations such as CIGR (International Commission of Agricultural Engineering) ,ESA (European Society of Agronomy) ,FAO (Food and Agriculture Organisation of the United Nations) ,

ICID (International Commission on Irrigation and Drainage) ,IUSS (International Union of Soil Sciences) , and others.

The scientific activity of Daniele deals with the following fields of interest: water resources management ,irrigation and drainage technology, performance assessment of sprinkler irrigation systems ,modelling of transport processes in porous media ,modelling and fluid-dynamics of debris and hyper-concentrated flows, flood control and mitigation measures, desertification and environmental impact of climate change, classical and quantum fluid-dynamical trajectories

Listed on :

- *Who's Who in the World ,23rd,24th,25th Editions ,Marquis (USA) Editor ;*
- *Dictionary of International Biography ,33rd ,34th , International Biographical Centre (UK) Editor;*

- *2000 Outstanding Intellectuals of the 21st Century , Fifth Edition ;*
- *Great Minds of the 21st Century , 2006/2007 Edition , American Biographical Institute , USA*

Water Droplet Trajectories in an Irrigation Spray: the Classical and Quantum Mechanical Pictures

D. De Wrachien, G. Lorenzini, S. Mambretti

40th International Symposium on Actual Tasks on Agricultural Engineering
Opatija , Croatia , 21-24 February 2012, pg 85-96

Abstract

A throughout understanding of the factors affecting spray flow in irrigation systems is important for developing appropriate conservation strategies. Resolving this problem involves both theoretical and experimental considerations.

Among the theoretical studies the classical mechanical approach, based on Newton's law, offers a useful tool to describe the trajectories of water droplets travelling from the sprinkler nozzle to the ground. Within this context, a mathematical model for irrigation sprinkler droplet ballistics has been presented and validated. Moreover, a new approach has been proposed, the so-called quantum mechanical picture based on the time-dependent Schrödinger equation and the wave function. This procedure leads to a new concept of quantum ballistics, in analogy to the well-established concept of classical trajectory, and represents a versatile tool for the description of the motion and of the dynamical properties of falling particles, as well as an exciting area of research in the years to come.

Introduction

A quantitatively reliable description of water droplet trajectories in sprinkler irrigation practice is a challenging task. Resolving this complexity involves both theoretical and experimental considerations. For an analytical picture of the process, the mutual dependence of the parameters characterizing the phenomenon (such as: dimension of the droplet, air friction, wind velocity) needs to be identified and properly described by the hydro-dynamical equations representing water spray trajectories. The issue entails both experimental and theoretical studies. The aim of the former is to identify, and so to measure, the contribution of each parameter to the final result; the target of the second is to work out an exhaustive analytical framework of the process. Both experimental and theoretical attempts in this field have been brought forth recently, but still the word "end" is far from being given. With reference to the subject, two physical-mathematical approaches to water droplet ballistics are presented and analyzed in this work. The first application involves the classical mechanical picture of the water droplet trajectories; the second one is based on quantum mechanics and on the time-dependent Schrödinger equation.

The future of irrigated agriculture between opportunities and threats

Journal Irrigation & Drainage Systems Engineering Editor Note Volume 9 Issue 2 (2020)

Daniele De Wrachien, Marco Medici

The role played by irrigated agriculture

Irrigated agriculture is expected to continue to play a major role in achieving

sustainability in the food and agriculture sector, through improvements towards food security and quality of life, while conserving the environment.

Especially during the second half of the last century investments in water for agriculture have made a relevant contribution towards sustainability by promoting decent livelihoods, increasing food security and reducing poverty. From 1940s food production started to outpace population growth, with an average annual crop production growth of 2.0-2.1% over the period 1969–1999. Higher yields have been partially achieved due to the expansion of irrigated areas and improvements in water management on irrigated lands.

Over the same period irrigation development has increased food stability, lowered food prices, created employment opportunities and increased rural income, with a multiplier effect estimated as between 2.5 and 4. The prevailing point of view is that the impacts of irrigation have been much more significant than simply agricultural development, embracing relevant rural developments, transforming road systems, education, health, and the entire way of life in rural areas.

Today, irrigated agriculture has to cope with a number of threats and challenges such as water scarcity, mitigation of negative environmental impacts associated to conventional agriculture, with the opposition of climate change effects.

Any increment of agricultural yields will necessarily rely largely on site-specific approaches characterized by not only a more accurate estimation of crop water requirements, but also on improvements in operation and management of irrigation and fertirrigation practices.

Problems and threats

Global land and water resources are considered to be sufficient to produce food over the next 50 years on the condition that water for agriculture is better managed. But which factors will reshape the future of irrigation and drainage systems?

Today a number of countries are economically constrained and in the condition of not continuing financing irrigation and agricultural research. The decline of public expenditure may bring unpleasant consequences such as economic stagnation, increases in world food prices and further degradation of the agricultural resource base.

A second point relates to production trends. According to future projections in developing countries the share of irrigation to total agriculture production is expected to relevantly increase as global population shift from staple crops to higher value food produce. This trend is associated with investments in food supply chain reliability and precision water application, as already demonstrated in China.

In addition, by 2050 approximately two-thirds of the world's people will live in cities (UN 2018). The increasing urbanization will in turn increase water demand, stressing competition between urban and agricultural sectors, and changes the production structure of agriculture.

Thereby, technological improvements capable of increasing the productive capacity of agriculture need to be encouraged at both institutional and private level. The present irrigation infrastructure is deteriorating or aged and need to be preserved and modernized. Water applied has to be maximized, limiting losses and re-using low-quality water effluents: investments are required to improve the existing infrastructure. To balance future water demand shifted by urbanization processes, compensating investment in new supplies and increased water productivity will be required. Also, additional investments in water treatment and conveyance will be necessary in order to reuse urban and industrial wastewater in agriculture.

How irrigation and drainage systems will have to adapt to climate changes are issues

that institution are compelled to cope with. Climate change represents somehow additional uncertainty towards the scope for increasing water productivity and may additionally hamper the availability of water resources as one of the main concerns regards increased rainfall variability. Reductions in rainfall at tropical latitudes have been already observed, while irrigation water withdrawals are currently stressing many of the world's major river basins.
Other possible impacts of climate variability include changes in temperature, sea level rise, floods and coastal erosion.

Possible responses

The aforementioned contingencies may affect planning principles and design criteria which will have to be systematically reviewed, with increased flexibility in planning and design processes in order to incorporate uncertain responses to the various possible climate impacts. Short-term strategies need to be implemented to face long-term uncertainties. Effective programs would have to be implemented within the following contexts:

- Increased stakeholder participation, including governments, professional and research institutions and non-governmental organizations to action programs at international (river basin), national, and regional level
- Raising expenditure on irrigation and agricultural research, avoiding stagnation and increases in food prices and containing degradation of the agricultural resource base
- Adoption of a comprehensive integrated approach for environmental management of water and land, improving water control capability in terms of quantity and quality

Enhanced water supply predictability and increase transparency and accountability to the final user, with water pricing based on measured deliveries.

Implications of distributed ledger technologies on firm cost structure and supply chain integration

Journal of Agricultural Research ,Volume 5 , Issue 2, 2020

Marco Medici, Daniele De Wrachien, Maurizio Canavari

Introduction

Technological infrastructures based on distributed ledger technologies (DLTs) like blockchain technology (BCT) are new digital technologies combining peer-to-peer networking and cryptography to create immutable public ledgers characterized by decentralization, collective maintenance, consensus trust and reliable data. DLT, today considered as an interdisciplinary topic, is expected to transform current economic organization and governance, and can be considered one of the evolutionary next steps for agriculture, particularly for current state-of-the-art of precision agriculture.

From the economic perspective, infrastructures based on DLT depict favourable conditions to lower transaction costs for the enterprise adopting such technology, through costless verification and without the need for costly intermediation.

Even though the DLT application to agriculture is somehow underachieved, it would be interesting to understand how such technology adoption in agriculture can re-shape firm boundaries. Investigating the extent to which the single firm can increase its integration with other sellers and buyers of the value chain, both in the view of the single actor and a whole value chain perspective, is extremely important.

Global warming effects on irrigation development and crop production. A world-wide view

Daniele De Wrachien, Mudlagiri B. Goli

Journal Agricultural Sciences, Vol. 6 No.7 , July 31,2015

Abstract

Despite the enormous advances in our ability to understand, interpret and ultimately manage the natural world we have reached the 21st century in awesome ignorance of what is likely to unfold in terms of both the natural changes and the human activities that affect the environment and the responses of the Earth to those stimuli. One certain fact is that the planet will be subjected to pressures hitherto unprecedented in its recent evolutionary history.The "tomorrow's world" will not simply be an inflated version of the "today's world", with more people, more energy consumption, more industry, rather it will be qualitatively different from today in at least three important respects.

First, new technology will transform the relationship between man and the natural world. An example is the gradual transition from agriculture that is heavily dependent on chemicals to one that is essentially biologically intensive through the application of bio-technologies. Consequently, the release of bio-engineered organisms is likely to pose new kinds of risks if the development and use of such organisms are not carefully controlled.
Second, society will be moving beyond the era of localized environmental problems. What were once local incidents of natural resource impairment shared throughout a common watershed or basin, now involve many neighboring countries. What were once acute, short-lived episodes of reversible damage now affect many generations. What were once straightforward questions of conservation versus development now reflect more complex linkages.

The third major change refers to climate variations. It is nowadays widely accepted that the increasing concentration of the so-called greenhouse gases in the atmosphere is altering the Earth's radiation balance and causing the temperature to rise. This process in turn provides the context for a chain of events which leads to changes in the different components of the hydrological cycle, such as evapotranspiration rate, intensity and frequency of precipitation, river flows, soil moisture and groundwater recharge. Mankind is expected to respond to these effects by taking adaptive measures including changing patterns of land use, adopting new strategies for soil and water management and looking for non-conventional water resources (e.g. saline/brackish waters, desalinated water, and treated wastewater).

All these problems will become more pronounced in the years to come, as society enters an era of increasingly complex paths towards the global economy. In this context, engineers and decision-makers need to systematically review planning principles, design criteria, operating rules, contingency plans and management policies for new infrastructures. In relation to these issues and based on available information, this report gives an overview of current and future (time horizon 2025) irrigation and food production development around the world. Moreover, the paper analyses the results of the most recent and advanced General Circulation Models for assessing the hydrological impacts of climate variability on crop requirements, water availability and the planning and design process of irrigation systems. Finally, a five-step planning and design procedure is proposed that is able to integrate, within the development process, the hydrological consequences of climate change.

Passivity: The Key to our Reactive-Metals-Based Civilization

by Digby D. Macdonald, Member EUAS

Short Biography

Professor in Residence, University of California at Berkeley, 1/2013 – present; Distinguished Professor of Materials Science and Engineering, Penn. State Univ.,6/2003 – 12/2012; Vice President, Physical Sciences Division, SRI International, Menlo Park, CA, 1/98 – 7/99; Laboratory Director, Mat. Research Lab., SRI International, Menlo Park, CA, 4/87 – 7/91; Laboratory Director, Chemistry Laboratory, SRI International, Menlo Park, CA, 3/84 – 4/87; Director and Professor, Fontana Corrosion Center, Ohio State University, 3/79 – 3/84.

Awarded the 1991 Carl Wagner Memorial Award from The Electrochemical Society; The 1992 Willis Rodney Whitney Award from NACE; the W.B. Lewis Memorial Lecture by Atomic Energy of Canada, Ltd., 1993, "in recognition of [his] contributions to the development of nuclear power in the service of mankind"; Elected Fellow, NACE-International, 1994; Member, USAF Scientific Advisory Board, Protocol Rank: DE-4 (Lieutenant General equivalent), 1993-1997; Elected Fellow, The Electrochemical Society, 1995; Royal Society of Canada, 1996. ("National Academy" of Canada); Royal Society of New Zealand, 1997. ("National Academy" of New Zealand); H. H. Uhlig Award, Electrochemical Society, 2001; U. R. Evans Award, British Corrosion Institute, 2003; Fellow, Institute of Corrosion (UK), 2003; Elected Fellow, World Innovation Foundation, 2004; Fellow, ASM International, 2005; Fellow, International Society of Electrochemistry, 2006; Khwarizmi International Award Laureate in Fundamental Science, Feb. 2007; Trustee, ASM International, 2007-2010; SABIC Visiting Chair Professor, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, 2010; Lee Hsun Research Award, Chinese Academy of Sciences, China, 2010; Inducted Doctuer Honoris Causa by INSA-Lyon, Lyon, France, 2011; Nominated for the 2011 Nobel Prize in Chemistry; Faraday Memorial Trust Gold Medal, 2012; Gibbs Award in Thermodynamics by IAPWS, 2013; Awarded Frumkin Medal, ISE, 2014; OLIN Palladium Medal by the Electrochemical Society, 2015; Ad Augusta Award from Auckland Grammar School, 2016.

The phenomenon of passivity is the enabler of our metals-based civilization, because it allows the use of reactive metals (Fe, Mg, Al, etc) and their alloys to be used in fabricating machines that are in contact with terrestrial environments. The topic has been one of intense scientific interest from the time of Schönbien and Faraday in the mid-1830s. At that time, Faraday speculated that the passivity of iron in nitric acid was due to the formation of an ultra-thin, invisible oxide layer on the metal surface that effectively separates the reactive metal from the corrosive environment. This "passive" film reduces the corrosion rate to a level that enables these materials to be used in engineering structures with tolerable changes in dimension upon their reaction with the environment (i.e., "corrosion"). Thus, aluminum has an energy density that is about the same as that of jrt fuel, yet we fly through the air in machines that are fabricated from the former and are powered by the latter. Why is that possible? Why doesn't the aluminum aircraft simply burn?

Little progress was made since the time of Faraday and the subsequent work of Verwey (1930s) and Mott (1940s, Nobel Laureate in Physics in 1977 for work on electronic structure of magnetic and disordered systems) in understanding passivity. Over the past thirty years, in an oft-cited series of papers, Professor Macdonald described his intensive and extensive investigations of the phenomenon of passivity, with the goal of developing a theory and *deterministic* model that could account quantitatively for the phenomenon of passivity and that might be used to design new alloy systems exhibiting superior corrosion resistance in industrial service. The outcome of this effort was the *Point Defect Model* (PDM). The PDM represents a dramatic, revolutionary departure from previous theoretical constructs (theories and models) has no known conflicts with experiment. Indeed, the PDM has predicted new (previously unknown) phenomena associated with passivity and passivity breakdown, ranging from photo-inhibition of passivity breakdown (PIPB), to resistive depassivation, to the design of new corrosion-resistant alloys (CRAs) at the atomic level. The PDM provides, for the first time, a realistic, testable explanation of why certain alloying elements, such as molybdenum or tungsten, when added in small amounts (< 5 at. %) to stainless steels, for example, dramatically enhances the resistance of the steel to passivity breakdown in chloride-containing environments, such as seawater.

Many decades of careful work using the most sensitive surface analysis techniques by a great number of researchers has revealed that passive films form as bi-layer structures, comprising a defective "barrier" oxide or hydride layer adjacent to the metal and a precipitated out layer formed by the hydrolysis of cations that are transmitted through the barrier layer. This is evidenced by the fact that species in the environment are generally present in the outer layer but not in the barrier layer, but species present in the alloy are found in both layers. The key to defining the properties of the passive film and hence in the development of the PDM is understanding the point defect structure of the barrier layer. Mott-Schottky analysis reveals that the defect concentration in the barrier layer is very high (10^{20} – 10^{22} cm^{-3}), an observation that can only be accounted for by postulating that defect generation and annihilation reactions occur at the metal/barrier layer (m/bl) and barrier layer/solution (bl/s) interfaces, in close juxtaposition (1- 3 nm) . Thus, the picture that emerges is that the barrier layer is a degenerately-doped, defect semiconductor with the dopants being cation vacancies (electron acceptors, most prevalent near the barrier layer/solution interface) and oxygen vacancies and metal interstitials (both electron donors and both most prevalent close to the metal barrier layer interface). From an electronic viewpoint, therefore, the barrier layer is best described as a metal/n^+ - i - p^+/solution structure, with the relative p vs. n character depending upon the relative concentrations of the electron acceptors and donors in the layer. Thus, the $Ni_{1-x}O_{1-y}$ barrier layer on nickel metal is p-type and is best described as a metal/n - i - p^+/solution structure, because x >> y, On the other hand, in the case of the barrier layers on iron and chromium, represented by $Fe_{3-x+z}O_{4-y}$ and $Cr_{2-x+z}O_{3-y}$, respectively, where x and z define the cation deficiency and cation excess in the barrier layer lattice, are best described as (Fe, Cr)/ n+ - i - p/solution structures, because x + y >> z. Thus, the closest classical electronic structure to that of a barrier layer is that of a tunnel diode (invented by Reona Esaki, Nobel laureate, 1973, for work on electron tunneling).

Amongst the more important predictions of the PDM is that, if the barrier layer is n-type in electronic character, the steady-state passive current density should be independent of voltage, whereas if the layer is p-type, the logarithm of the passive current should increase linearly with voltage, provided that no change in the oxidation state occurs upon ejection of a cation from the barrier layer into the solution. If a change in oxidation state of the cation does occur, the logarithm of the passive current density is predicted to increase or

decrease with increasing voltage, depending upon the sign of the oxidation state change. The PDM also predicts that the thickness of the barrier layer increases linearly with the applied voltage, regardless of the electronic character, and that the passive current, in the case of iron, zinc, and chromium, is carried primarily by cation interstitials. On the other hand the passive current of nickel and tungsten is due to the transmission of cation vacancies and oxygen vacancies, respectively, through the barrier layer. These predictions are all observed over many systems, with no exceptions.

One of the revolutionary postulates of the PDM is the postulate that the *electric field strength within the barrier layer is independent of applied potential and barrier layer thickness*. This hypothesis is based upon the phenomenon of Esaki tunneling, which buffers the field strength in thin depletion regions of highly doped semiconductor structures. This hypothesis is diametrically opposed to that of the classical Verwey, "high-field" model and to that of the Cabrera-Mott variant of the classical model, which assume that the field strength decreases as the film thickens at constant voltage. The latter models cannot explain the linear dependence of the film thickness on applied voltage or account for the finite steady-state current density in the absence of a redox acceptor in the solution. Furthermore, the classical model predicts electric field strengths for very thin oxide films that are well above the dielectric strength of the defective oxide barrier layer and hence should result in dielectric breakdown and sparking. This is not observed.

If passivity was perfectly protective of a reactive metal in contact with a corrosive environment, corrosion would not exert the enormous cost on society that it currently does. Thus, studies have shown that the cost of corrosion in an industrialized society is about 4.5% of the GNP. In the US this amounts to about $945 billion or about $3000 per man, woman, and child in the nation, annually, based on the current GNP of $21 trillion. The great majority of this cost is due to passivity breakdown, which is essentially nature's mechanism for returning the reactive metals to the natural states (ores) from which they were so laboriously won by mining, smelting, electro-winning, or chemical reduction. Nature's principle agent for affecting this process is the chloride ion (Cl^-), which is ubiquitous in terrestrial environments. While many other anions induce passivity breakdown, by far the most aggressive is chloride. Thus, in another remarkable series of papers over the past thirty years, Professor Macdonald, using the PDM, unraveled the mysteries of passivity breakdown. In doing so, he and his colleagues have further developed the PDM to explain a variety of phenomena associated with passivity and passivity breakdown, including: (i) The nucleation of pits, including the distributions in the critical breakdown voltage (V_b) and the inductor time (t_{ind}), (ii) the dependencies of V_b and t_{ind} on the concentration of aggressive ion in the environment (typically Cl^- for iron and nickel based alloys), (iii) photo-inhibition of passivity breakdown (which was discovered by Macdonald in 1985), (iv) the role of alloying elements (e.g., Mo, W) in inhibiting passivity breakdown, (v) erosion/corrosion, (vi) the segregation of alloying elements into the passive film, and (vii) depassivation. The PDM has now been tested extensively (not only by Professor Macdonald, but also by many others), and it has been found to account quantitatively for all passivity breakdown phenomena when quantitative tests have been devised. Of particular importance is the prediction of the PDM is that light of sufficiently high photon energy should inhibit passivity breakdown by quenching the electric field. Prof. Macdonald's research group demonstrated this phenomenon in 1985 for nickel in chloride-containing borate buffer solution and more recently for stainless steels and Cu/Ni alloys in similar environments. PIPB is now being developed as a practical corrosion control technology for protecting components in thermal power plant

steam cycle systems, all of which normally operate in the dark (inside pipes and vessels).

The role of chloride (and other halide ions) in inducing passivity breakdown has been a matter of considerable controversy for more than 100 years, with some explanations postulating that the anion penetrates the barrier layer. Largely through the work of Prof. Macdonald, it is known that penetration does not occur. On the other hand, through theoretical work by Prof. Macdonald and his students, it is evident that chloride catalyzes the generation of cation vacancies at the barrier layer/outer layer (solution) interface. The so-generated cation vacancies migrate across the barrier layer from the barrier layer/solution (bl/s) interface to the metal/barrier layer (m/bl) interface where they are, ordinarily, annihilated by injection of a cation from the underlying metal. Professor Macdonald demonstrated theoretically that absorption of chloride anions into oxygen vacancies at the bl/s interface results in an enhanced flux of cation vacancies across the barrier layer. Because the annihilation reaction at the m/bl interface has only a limited capacity to annihilate cation vacancies, the excess vacancies in the enhanced flux condense on the cation sublattice or on the metal lattice at the m/bl interface, thereby causing the barrier layer to locally separate from the metal and form a nano-scale blister Because film growth into the metal requires intimate contact between the metal and the film, penetration of the film into the metal beneath the blister stops, but it still occurs at the periphery, where intimate contact exists. However, the film continues to dissolve at the bl/s interface so that the "cap" of the blister thins and fractures under the action of film growth stresses. This marks a meta-stable breakdown event. By assuming that a large population of such sites exist on a real metal or alloy surface, and by postulating that these sites are normally distributed with respect to the cation vacancy diffusivity in the barrier layer, because the breakdown sites are sites of local lattice disorder, it is possible to derive mathematical expressions for V_b and t_{ind} and for the distributions in these quantities. Excellent agreement with experiment leaves little question as to the validity of the theory and model.

Prof. Macdonald and his colleagues have combined electrochemical impedance spectroscopy (EIS) and passivity breakdown studies to ascertain the role of chloride ion in the nucleation of meta-stable pits on nickel in chloride-containing solutions. EIS was used to determine rate constants for the vacancy generation and annihilation reactions and for barrier layer dissolution by optimizing the PDM on the impedance data. It was found that the rate constants of reactions at the metal/barrier layer interface were unaffected by chloride ion, as were reactions involving film dissolution and oxygen vacancy annihilation at the film/solution interface. These findings eliminate chloride penetration and film dissolution as mechanisms for passivity breakdown on nickel. Instead, the data show that the cation vacancy generation reaction occurring at the film/solution interface is catalyzed by chloride ion in a first-order manner leading to a great increase in cation vacancies in the film, as determined by Mott-Schottky analysis. *This finding is in complete accord with the PDM and provides a direct demonstration of the ability of the PDM to describe passivity breakdown, at least in the case of nickel.* This same mechanism of passivity breakdown has now been demonstrated for a large number of metals and alloys, with no exceptions.

The goal of deterministically predicting the evolution of corrosion damage has largely been achieved and is embodied in the protocol Damage Function Analysis (DFA). DFA has been employed to predict the evolution of general and localized corrosion damage to canisters for the disposal of High-Level Nuclear Waste (HLNW), for example.

Investigation of the Loss of Capacity in Stretched Plates with Defects

by Nikita Morozov, Member EUAS

Short Biography
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When designing load-bearing structures, particular attention should be paid to the zones characterized by high stress levels and gradients, which are critical to the durability and reliability of the structure, with negative aspects affecting the performance of structural elements being both their possible destruction and loss of stability.

Since the 1970s, active studies of the local stability of plates with defects such as cracks and notches under tension have begun. The studies encompassed the problems of displacements in the direction perpendicular to the plane of the plate and their development with the increasing of tensile load observed when a certain critical load is reached. Dixon J.R., Stranningan J.S. (1969), Yu.M. Dahl (1978), Markström K., Storäkers B. (1980), A.N. Guz, M.Sh. Dyshel, G.G. Kuliev, O.B. Milovanova (1981), Sih G.C., Lee Y.D. (1986) and others.

The resulting postcritical deformation state with local loss of stability near the indicated defects leads to a fundamental change in the geometry of the plate and, as a consequence, to a significant redistribution of stresses. In this regard, it is important to study the effect of this geometry change on fracture.

Solving this problem is a complex nonlinear challenge requiring nonlinear analysis using numerical methods. In recent decades, interest in these problems is due to the miniaturization of devices and structures using thin-walled nanoscale elements, the bending stiffness of which is low.

The effect of nanoscale thickness on the local buckling of cracked plates and on the stress intensity in the vicinity of crack tips, generated by a change in the plate geometry, has been studied.

Within the framework of the above-mentioned studies, it is proposed to

investigate the local instability of plates with defects under dynamic loading. Problems for plates with cracks and defects with corner points are of particular interest. Based on the results obtained during the study of the asymptotic behavior of solutions of dynamic problems in the vicinity of corner points (Kokotov A.Y., Plamenevskii B.A. *On the asymptotic behavior of solutions of the Neumann problem for hyperbolic systems in domains with conical points.* Algebra and Analysis. 2004. V. 16. No. 3. 477-506; S.I. Matyukevich, B.A.Plamenevsky, *On dynamic problems of the theory of elasticity in domains with edges*, Algebra i Analiz, 2006, Volume 18, Issue 3, 158–233), it is planned to study the influence of geometry defects on local stability of nanoscale plates under dynamic tensile loads.

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New Contributions in Atmospheric Propagation & Microwave Biophysics

by André Vander Vorst, Member EUAS

Short Biography

André Vander Vorst was born in Brussels in 1935. At high school, he studied classical humanities, including Latin and Greek. He graduated in 1958 as an electrical and mechanical engineer at the UC Louvain (UCL), Belgium, from which he received his Doctoral degree in 1965. During his thesis he spent six weeks working at Philips Natuurkundig Laboratorium, Eindhoven, The Netherlands. As a research associate, he was at M.I.T 1964-1965 where he received a M.Sc. degree in microwaves, and at Stanford University 1965-1966, both in radioastronomy. In 1966, he founded the Microwave Laboratory at UCL, which he headed for 35 years. His research interests were successfully loaded waveguides and cavities, atmospheric propagation up to 300 GHz, opto-microwaves, humanitarian demining, and bio-microwaves. He has been teaching in four Belgian Universities on electromagnetics, transmission lines, and microwaves. He also taught analogue and hybrid computation, antennas, and microwave and satellite communications. He supervised 27 doctoral theses and about 200 engineer's theses.

Prof. Vander Vorst has authored and co-authored seven books, a number of book chapters, and more than 300 papers in peer-reviewed journals and conference proceedings. His last book, RF/Microwave Interaction with Biological Tissues, with A. Rosen and Y. Kotsuka as co-authors was published by Wiley U.S.A. in 2006. He recently was co-author of papers on various websites on the 5G and the effect of electromagnetics on viral infections. He is now writing chapters on bioelectromagnetics in a collective book investigating electro-hypersensitivity.

Through his academic career at UCL, Prof. Vander Vorst has been Head of EE Department 1970-1971, Dean of Engineering 1972-1975, Vice-President of the Academic Council 1973-1975, and President of the Open School in Economic and Social Politics 1973-1987.

Over the last 50 years, Prof. Vander Vorst has been actively involved in developing the International microwave community. In 1967-2001 he was chairing Student Activities Committee and Educational Activities Committee and setting up Chapter Coordination Committee in I.E.E.E. Region 8. He was a corresponding member of the Organizing Committee of the first European Microwave Conference (EuMC) in London 1969, Chair EuMC Technical Program Committee in Brussels 1973, and Chair EuMC in Liège 1984. Ha has been a reviewer for every EuMC since 1969. He is a founder member of the European Microwave Association (EuMA) and has been EuMA Secretary General for 18 years. In the latter function he has set up and developed EuMA Headquarters. He is now appointed Secretary Emeritus and Data Protection Officer.

Prof. Vander Vorst has offered his service to the microwave community also under the umbrella of I.E.E.E. MTT Society, in which he has been active in 1985-2006. He is a Life fellow of the I.E.E.E. and obtained a number of awards including the Microwave Career Award 2004 from I.E.E.E MTT-S and the Propagation Award 2019 of the European Association for Antennas and Propagation (EurAAP).

He is an associate member of Belgian Academia of Letters and Science, a member of Academia Europaea, the Electromagnetics Academy, and EU Academy of Sciences. He is an Honorary Member of Belgian National Committee or URSI. He has been a member of National Health Council in both Belgium and The Netherlands.

He has been cited in a number of Who'sWho.

He loves music and has conducted choirs for more than 40 years.

He has five children and twelve grandchildren.

From 1960 to 1964, André Vander Vorst investigated fast switching of magnetic cores for his doctoral thesis. As a research associate with a post-doctoral fellowship, he spent two years in the USA: 1964-1965 at M.I.T. and 1965-1966 at Stanford University in both Laboratories of Radio-astronomy. In 1966, back in Belgium he founded the Microwave Laboratory at the Université catholique de Louvain (UCL). Some typical publications are mentioned in what follows for each research topic mentioned.

He started research on propagation in lossless closed structures at X-band like loaded waveguides and cavities. The first doctoral thesis he supervised in the Laboratory was by F. Gardiol, 1966-1969, who analytically investigated the impact of a one-dimensional inhomogeneity on waveguide propagation [1].

Simultaneously, A. Vander Vorst started developing numerical analysis for propagation in diverse inhomogeneously loaded microwave transmission lines by means of variational principles [2]. He produced a numerical version of the variation-iteration method presented by Morse and Feshbach, *Methods of Theoretical Physics*, Part 1 and 2, McGraw-Hill, 1953. In 1969, he obtained the first numerical solution of a second-order partial derivative eigenvalue equation, describing the propagation in a rectangular waveguide loaded by inserts.

A number of doctoral students then investigated the impact of inhomogeneity on miscellaneous propagating structures, like microstrips, fin lines, and p-i-n transmission lines, as well as opto–induced effects on transmission lines [3]-[8].

This research ended up with propagation on lossy distributed structures at frequencies up to 100 GHz. In 2002, he co-authored with I. Huynen a research book on variational principles and distributed circuits [9].

Atmospheric propagation has been a research interest of A. Vander Vorst from 1968 [10] until about 2000. In 1970, he set up two horizontal links at 11.6 and 35 GHz, respectively, operating for a five-year period [11]. This has been the subject of the first of his five consecutive COST projects on atmospheric propagation, covering both horizontal links and slant paths.

He was the Belgian participant to the Orbital Test Satellite (OTS) of the European Space Agency (ESA), 1978-1983. For this, he obtained significant funding from the Belgian State (equivalent to 5 million EUR at today's value) to obtain one transmitting-receiving fixed television station at 14 GHz (up, 2 kW) and 11 GHz (down), as well as two receiving stations at 11 GHz, one fixed and one mobile [12]-[14].

He has been, together with D. Vanhoenacker-Janvier, the Belgian participant to the ESA Olympus experiment, 1988-1993, and obtained significant funding from the Belgian State and PTT Department, respectively, to set up two receiving stations at 12.5 and 30 GHz and 12.5 and 20 GHz in both polarisations at both frequencies, respectively. Measurements made at Louvain-la-Neuve included attenuation, depolarisation and scintillation at 12.5 and 30 GHz and radiometry in two polarisations at 12 and 35 GHz [15]. Fast measurements were available, every 34 ms, especially in view of investigating the time scale of the scintillation effects.

These experimental tools stimulated original atmospheric propagation investigations in theory, experiment, and simulation as well. With the OTS stations, the Laboratory has been one of the three research centres to experimentally point out the microwave scintillation phenomena, extensively investigated by D. Vanhoenacker-Janvier in her doctoral thesis and later.

Site-shielding, in particular by a knife-edge obstacle, has been investigated with measurements from 8 to 94 GHz [16]. The research then evaluated the bit-error rate prediction of atmospheric communications links [17]. It continued until the year 2000 with the evaluation of some special effects related to the structure of linearly tapered slot antennas including the Vivaldi antenna, up to some tens of GHz [18].

A. Vander Vorst conducted research on atmospheric propagation of EM waves at frequencies up to 300 GHz [19]. He has been involved in EM wave propagation since 1960, start of his doctoral thesis, until the end of his active professional career.

Microwave biophysics has been another subject of interest of A. Vander Vorst. The project started at the end of the 70s by designing and implementing a system for eliminating bacteria in air by microwave heating, to proceed to open air medical surgeries. This system was patented and commercialized.

Experimental work has been going on with rabbits from 1987 through 1994, for the doctoral thesis by J. Teng, in three experimental steps. The first was devoted to developing a microwave acupuncture method by inserting a miniature cable into acupuncture points and exciting these by injecting microwaves in the cable, offering a quantitative method for measuring analgesia. The purpose was to excite the nervous system in some specific points for detecting an analgesic effect. Results were positive [20]. The second consisted of the development of a method to measure the

effect of analgesia in the cervical centre of pain [Fig. 1]. This showed that by doing so the composition of the cervical liquid in the pain centre was modified similarly to what is obtained when ingesting analgesic products [21].

In the third step, a method was developed for measuring in the cervical centre of pain the effect of an electric impulse applied to a rabbit's foot in both the absence and presence of analgesia produced by microwave acupuncture. Simultaneously, the deformation of the impulse was measured on the nervous system and in particular the spinal cord, by inserting a microwave micro-antenna inside of the backbone [22], looking for a non-thermal microwave effect. The result was negative [23].

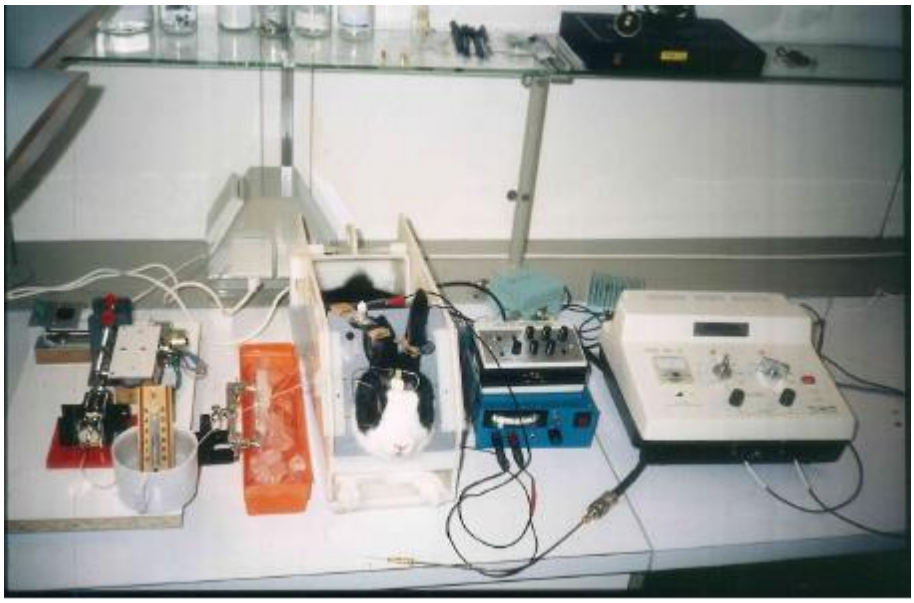

Figure 1. Measuring pain threshold on a rabbit as a function of antalgic microwave acupuncture

A cooperation went on with colleagues of the UCL School of Medicine in the years 1993-1997 to evaluate the effect of magnetic induction produced by a coil to implant on a mouse for obtaining a muscular reinforcement. The result was positive [24].

Dielectric parameters and blood absorption have been measured from 2 to 110 GHz [25] and a review of microwave effects on nervous system and nervous fibre has been performed [26].
Research has then been more oriented toward biological effects and medical applications [27] and more specifically to biological effects on living systems and especially human beings [28]. Face heating at the occasion of a telephone conversation has been measured in direct view of a base station, on stairs and in the basement of a building, respectively, with the measurement of an increase of 0.7°C after 10 minutes in the basement [29].

Specific very low frequency magnetic field measurements have been made on spontaneous bioelectric activity of neurons [30] while dielectric absorption microwave power has been evaluated at the scale of nucleic acids [31].

Microwave exposure of rats has been prepared, performed and evaluated from 1998 through 2009, for the doctoral thesis of D. Adang. Rats were submitted to a microwave level corresponding to the calculation by WHO of the limit for the human being, taking into account however a factor 10 for difference of length between the human being and the rat. The exposure duration has been long: 2 hours per calendar day of 70% of the rat lifetime which was 30 months. There were four groups of 31 rats, including three groups exposed to three different microwave schemes, respectively, and one sham-exposed group, with in particular exposure to 970 MHz CW. Fifteen

blood parameters were analysed 6 times on the 124 rats, yielding more than 10.000 biological data, together with behavioural effects and mortality. A combination of positive and negative results has been obtained on monocytes, behavioural effects, and mortality, respectively [32][33].

Planar antennas have been designed and evaluated in view of medical applications, from 2005 through 2013, being mainly the subject of the doctoral thesis of H. Halheit. This necessitated the evaluation of a radiating structure, the operating frequencies, the influence of the substrate on the resonance frequencies of the antenna and their bandpass, the power necessary for medical applications, and mutual coupling between the elements [34]. A number of presentations have been made in medical symposia [35].

At the request of Wiley, a research book was written on the subject of *RF/Microwave interaction with biological tissues* and published by Wiley U.S. in 2006, with PhD students as a prime target [36].

During the last years, A. Vander Vorst co-authored papers on various websites on 5G and on the effect of electromagnetics on viral infections. He is now writing chapters on bioelectromagnetics in a collective book investigating electro-hypersensitivity.

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Further Investigations in Flat Panel Technolgies

by Vladimir Chigrinov, Member EUAS

Short Biography

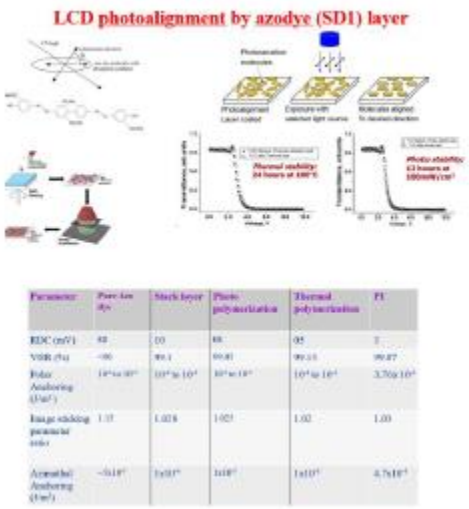
Professor Vladimir G. Chigrinov is Professor of Hong Kong University of Science and Technology since 1999. He is an Expert in Flat Panel Technology in Russia, recognized by the World Technology Evaluation Centre, 1994, and SID Fellow since 2008. He is an author of 6 books, 31 reviews and book chapters, about 313 journal papers, more than 662 Conference presentations, and 116 patents and patent applications including 35 US patents in the field of liquid crystals since 1974. He got Excellent Research Award of HKUST School of Engineering in 2012. He obtained Gold Medal and The Best Award in the Invention & Innovation Awards 2014 held at the Malaysia Technology Expo (MTE) 2014, which was hosted in Kuala Lumpur, Malaysia, on 20-22 Feb 2014. He is a Member of EU Academy of Sciences (EUAS) since July 2017. He got A Slottow Owaki Prize of SID in 2018 http://www.ee.ust.hk/ece.php/enews/detail/660. He is 2019 Distinguished Fellow of IETI (International Engineering and Technology Institute). http://www.ieti.net/news/detail.aspx?id=184 http://www.ieti.net/memberships/Fellows.aspx

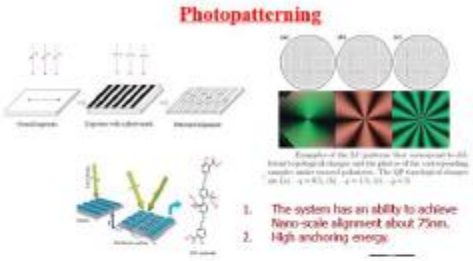
RESEARCH INTERESTS

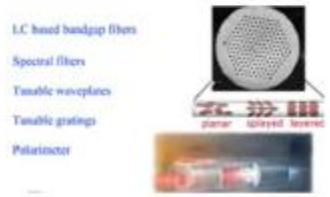
1. Computer modeling of various electrooptical effects in Liquid Crystals (LC).
2. Photo-aligning technique for LCD application.
3. LC devices in fiber optics.
4. Fast multistable ferroelectric LC devices.
5. LC applications in photonics.
6. LC devices for non-display applications.
7. Fast ferroelectric LC devices for field sequential applications.
8. New optically rewritable LC E-paper
9. LC based security films.
10. LC based smart windows.
11. Switchable LC antennas.
12. LC based sensors.

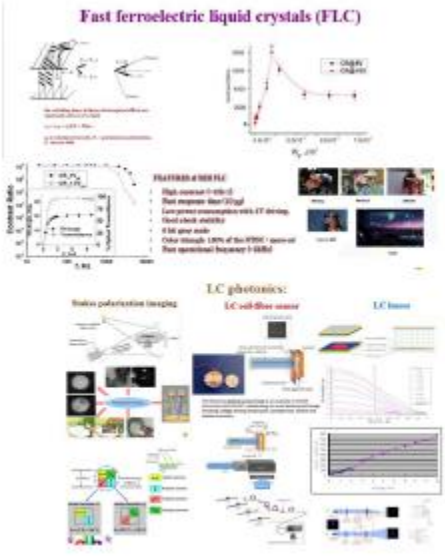
13. LC q-plates
14. LC lenses.
15. 100% patterned polarizers

The directions of research are shown below:









The following research has been done recently (year 2020)

1. Ma, Ying , Xin, Sang, Jing , Liu, Xiaoyu , Liu, Yang, Sun, Jiatong , Wang, Xiaoqian , Guo, Qi ,Chigrinov, Vladimir G., Colour generation for optically driving liquid crystal display, *Liquid Crystals*, Vol. 47, 7, pp.1-7 (2020).
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3. Qi Guo, Tian Liu, Xiaoqian Wang, Zhigang Zheng, Aleksey Kudreyko, Huijie Zhao, V. Chigrinov, and Hoi-Sing Kwok, Ferroelectric liquid crystals for fast switchable circular Dammann grating, *Chinese Optical Letters*, Vol. 18/8, pp. 080002 (1-4), (2020)
4. Vladimir Chigrinov, Jiatong Sun, Mikhail M. Kuznetsov, Victor Belyaev,and Denis Chausov, The Effect of Operating Temperature on the Response Time of Optically Driven Liquid Crystal Displays, *Crystals*, *10*, 626 (2020).
5. Vladimir Chigrinov , Jiatong Sun and Xiaoqian Wang, Photoaligning and Photopatterning: New LC Technology, *Crystals*, *10*(4), pp. 323-337 (2020)

Computer Aided Learning Machines

by Roger N. Anderson, Member EUAS

Short Biography

Roger retired emeritus after 42 years at Columbia University's Lamont Doherty Earth Observatory and Data Sciences Institute. Roger has led teams that have developed the next generation of machine learning control systems for smart hydraulic fracturing, 4D seismic reservoir simulation and smart energy management of electricity, water, steam and occupancy tracking for skyscrapers. ***In 2020, he was elected to the EU Academy of Sciences. Over his research career, Roger brought in more than a Quarter Billion $$ for Columbia University, including ship time costs.*** *He also co-founded AKW Analytics, Bell Geospace, 4D Technologies, CALM Energy and vPatch Inc. He co-invented 18 patents , with 8 more pending. Roger has had technical, business, computational, and working collaborations with Baker Hughes, Boeing, BBN, Booz, BP, Shell, Pennzoil, Con Edison, Range Resources, and has run consortiums with many others. Roger has been* ***in residence*** *at Baker Hughes, Con Edison Control Centers, the Earthquake Research Institute of the University of Tokyo, Fedex, Finmeccanica, GE, IBM Research, Kansas Geological Survey, KBR, Lockheed Martin, Rudin Management, Schlumberger, Sinclair, the Texas Energy Center, the Urban Utility Center of NYC, the United States Geological Survey, the University of California Berkeley and the University of Hawaii Manoa.*

Roger has written 7 books, edited 4 others, published more than 640 scientific and engineering papers, and written and produced 15 technical videos. While at Columbia, Roger graduated 9 Ph.D. students, many of whom are now leaders in national scientific and engineering communities like the National Environmental Research Laboratory, University of Illinois, Chicago, the US Geological Survey as well the international business communities Head of IBM Research Brazil, CNRS Marcelles FR, IT director of the Commodities Trading Floor at Citibank, and Head of Risk Management Software Development for PEMCO.

Roger's team was recently chosen as the winning University Program in General Electric's Ecomagination Innovation Challenge, winning a $1.2 million prize. While at the Lamont-Doherty Earth Observatory of Columbia, he founded the Borehole Research, Global Basins, 4-D Seismic, Seismic Reservoir Simulation, Portfolio Management and Energy Research Groups. Roger has been Chief Scientist of more than 20 oceanographic cruises, including in 1979, the first U.S. research ship to visit the Peoples Republic of China in the modern era. The Wall Street Journal recently characterized him as "a computer-imaging pioneer". ***However, perhaps his most difficult assignment ever was as Head of Umpires for many years at West Side Little League Baseball in Manhattan, NY.***

Fields of Interest

Research, Development & Deployment of Smart Infrastructure, Smart Electric Grid, Smart Building and Smart Cities Control Systems, Total Property Optimization, Smart Electric Vehicle Fleet Charging, Forecasting Package and Manufacturing Loads, Lean Energy Management, Real Options, Portfolio Management, Petroleum Reservoir Management, Alternative Energy Research, 4D Earth Imaging using Seismic & Gravity Gradiometry, Logging, Earthquake Stress Measurements, and Hydraulic Fracturing.

Education

Ph.D. Earth Sciences, Scripps Institution of Oceanography, University of California, San Diego, 1973. M.S. Geophysics, University of Oklahoma, thesis at Woods Hole Oceanographic Institution, 1971. B.S. Geophysics, University of Oklahoma, 1969.

Permanent Position

Emeritus Professor and Senior Research Scientist, Columbia University, 1974-Pesent.

Forty percent of all the energy **usage** in what we call "vertical cities", such as the great mega-cities of New York, London, Shanghai, Beijing, Hong Kong, Singapore, Delhi, Moscow, Berlin, Paris, and Tokyo, to name just a few, is consumed in producing the comfort and safety of tenants in high-rise office and apartment buildings. In turn, forty percent of energy **costs** in these buildings go to maintaining and operating the HVAC air conditioning and heating systems. High-Rise city buildings are obligated to provide comfortable spaces for the tenants that they house. The operation of these skyscrapers is in great need of energy optimization. Large buildings also occupy a very important information space, affecting the decisions of local governments and power-grid companies, as well as providing necessary services of security, water, and sewage, as well as power and digital infrastructures such as fast and uniformly available Internet for all. As the world has moved into the big-data **Computer Aided Learning Machine (CALM)** era**, Artificial Intelligence and Machine Learning** (AI/ML) are utilized by us to optimize and build more secure and efficient **energy** systems.

The need is not only for large urban buildings, but also for university campuses, military bases, hospitals, industrial and manufacturing facilities. But energy efficiency must be accompanied by improved productivity that sustains **clean**, comfortable and safe operating environments. We a patented AI/ML system-of-systems approach that requires that each building, campus, etc. must be treated as if it were like an organism, with data sensors providing **innervation** throughout all critical components. A central **brain** is then needed to provide the identification of problems, evaluation of possible solutions, and prioritization of actions—all in real time (see Refs for our CALM Book and Patent links).

In the even bigger picture, converting our cities to electric transportation systems is needed to fight **climate-change**. That requires conversion from gasoline and diesel service stations to electric recharge sites and e-parking garages. That, in turn, requires the electric grid to deliver more and more electricity with ever more efficiently to cities in environmentally and carbon neutral ways. That, in turn, requires massive, renewable electricity sources such as wind and solar farms with huge battery backup for when the wind does not blow and the sun does not shine, as well as new intelligent transmission lines. That, in turn, requires integration with distributed generation and storage facilities, such as photovoltaics on every rooftop and Universal Power Supply (UPS) type batteries in every garage. That, in turn, requires integration of the electric grid with other vital infrastructures like transportation, gas, water and sewage because electric pumps are critical to all these systems. That, in turn, requires all cities to modernize the entirety of their infrastructures, and all that must be integrated into a smart AI/ML system-of-systems with enough controls, monitors, intelligence, and above all physical and cyber security. That, in turn, requires all this to be placed **underground** so that the larger and more frequent hurricanes and wild-fires accompanying Climate-change do not take out the electricity so that the power must never go out.

My lab has been working for 40 years on this CALM AI/ML computational learning system-of-systems for energy optimization of all kinds. First and foremost, CALM's AI/ML methods must be used throughout, effectively combining many sources of information to derive predictions of outcomes from past, present and future performance forecasts. Advantages of AI/ML over traditional statistical methods include the ability to take into account redundancy among various sources of data in order to minimize the number of attributes that need to be monitored for real-time assessment and prediction, all the while re-ranking importance functions in a reasonable amount of computer time for

even the largest of data sets.

Modern ML methods such as Support Vector Machines (SVM), Deep Learning (DL), and Martingale Boosting (MB) have largely replaced earlier methods such as Artificial Neural Networks (ANN). The modern methods have significant advantages over the earlier ones. For example, ANN requires extensive engineering-by-hand both in deciding the number and arrangement of neural units and in transforming data to an appropriate form for inputting to the ANN, whereas SVM, DL and MB do not. The financial, medical, aerospace, and consumer marketing worlds have already adapted CALM AI/ML techniques and we are working to convert the energy industry as well.

AI/ML analyses of the sequence of changes over time of dynamic variables is an important additional determinant for root cause analysis in the CALM we have constructed at Columbia. Magnitude and rate of change of the variables can be used to derive the characteristics leading up to failure of a group of objects so that precursors can be recognized for the overall AI/ML system-of-systems. For example, dynamic variables are important in fields such as aerospace, where airplane take-off and landing cycles are more critical predictors of equipment failure than hours in the air. As these dynamic, time varying attributes are added to the AI/ML analysis, new solution plans can be re-calculated every time new data updates occur, and the differences between past solutions and predictions analyzed. Over time, the results migrate from prediction to control as the system learns how to optimize itself.

Examples of successful AI/ML abound in medicine and transportation, in particular. Consider the progression from storing patient medical records to synthesizing patient data to reach a machine-driven diagnosis. Also consider the progression from flight simulators that train pilots in how to fly to flight controllers that fly the plane on their own – we have even worked on an Unmanned Combat Air Vehicle (UCAV) that can successfully dogfight. Other successes are in the progression from speech recognition to synthetic speech conversation, and from driver aids such as navigation and a car that can park itself, to completely automated cars and trucks that require no human presence at all.

Reinforcement Learning (RL) is a difficult problem because the learning system must continually perform actions and be scored on whether that action was good or bad. For example, the AI/ML system flying the UCAV might be trained in a simulator and told not to crash. It will have to make many decisions each second and then, after acting on thousands of decisions, the aircraft might indeed crash anyway. What should the system learn from this bad experience? Which of its many actions were responsible for the crash? Assigning blame to individual actions is the problem that makes RL difficult. Luckily, there is a solution to this problem, called **Adaptive Dynamic Programming** (ADP). ADP is widely considered the most feasible way of solving general stochastic optimization control problems. However, it suffers from ``the curse of dimensionality," meaning that its computational requirements grow exponentially with the number of state variables.

The final required piece of the CALM system that we have built for energy optimization is **Adaptive Stochastic Control** (ACS). Techniques for generating a dynamic treatment control policy for a cyber-physical system have many components, including a collector for gathering data representative of the cyber-physical system, and an ASC including a combination of all the CALM techniques discussed above that are used to create the real-time **Brain** for generating predictions corresponding to available actions based on an objective function, and an ADP element configured to receive actual operational metrics. The ADP element learns the state-action map and generates dynamic treatment control policies using all AI/ML created models. ADP systems automatically adjust themselves to have performances which are optimal according to preassigned criteria. In our case we

build integrated real-time energy systems involving the use of models and simulators. For example, we have built all the above into an easy to use, stand-alone Electric Grid Analytics Learning Machine (EGALM). EGALM is a "brutally empirical" analysis system that integrates data across all relevant subsystems and finds "clusters" of correlation that differentiate high versus low efficiency performance for all scales of the electric grid. The objective of EGALM is to become the go-to **Brain** for all electricity operations. EGALM was reduced to practice after we patented the Petroleum Analytics Learning Machine, (PALM™), which analyzed more than 100 attributes integrated from all available data from more than 150 horizontal oil and gas wells from the Marcellus shale in Pennsylvania and the Permian Basin in Texas. EGALM is similarly a data-centric, computational learning and predictive analysis system that uses open source algorithms and unique techniques applicable to all electricity operations in the United States and other countries. Also, we have also built an Energy Analytics Learning Machine (EALM) for broader energy systems integration adding water, sewage, and digital communications systems required to run the cities of the world. Energy companies have never before been able to rigorously integrate and simultaneously analyze and optimize all the diverse data from the city to state and national electric grids, from the 6000+ power plants to the 700,000+ miles of transmission lines, to the countless transformers, substations, relays, feeders, and other data generating parts of neighborhood, city, and rural energy systems that power our modern economy.

These have led to the writing of a CALM book and have granted several US Patents that give further details of our technologies. The links to which are included in the **Refs** below. In addition, over 1550 pdf's of my scientific publications, sorted into 24 Research Projects, are available for free download at https://www.researchgate.net/profile/Roger_Anderson20

References

BOOK: Anderson, R. N., Boulanger, A. Johnson J., and Kressner, A., **COMPUTER AIDED LEAN ENERGY MANAGEMENT**, Pennwell, Publishing, 2008. http://books.google.com/ebooks?id=jvIbpdTj9XoC&dq=roger%20n%20anderson&as_brr=5&source=webstore_bookcard .

PATENTS AND AI/ML SOFTWARE AVAILABLE FOR NON-EXCLUSIVE LICENSING FROM COLUMBIA UNIVERSITY TECHNOLOGY VENTURES:
http://techventures.columbia.edu/industry/start-licensing-process

PATENTS GRANTED:

1. PETROLEUM ANALYTICS LEARNING MACHINE SYSTEM WITH MACHINE LEARNING ANALYTICS PRODUCTS FOR THE UPSTREAM AND MIDSTREAM OIL AND GAS INDUSTRY, **https://patents.google.com/patent/US10430725B2/en?oq=US10%2c430%2c725 .**

2. ENERGY ANALYTICS LEARNING MACHINE SYSTEM**,** https://www.researchgate.net/publication/339540811_Energy_Analytics_Learning_Machine_EALM .

3. ELECTRIC GRID ANALYTICS LEARNING MACHINE SYSTEM**,** https://www.researchgate.net/publication/342601902_EGALM_Patent_06302020 .

4. DYNAMIC CONTINGENCY AVOIDANCE AND MITIGATION SYSTEM**,** https://patents.google.com/patent/US10229376B2/en?oq=US15%2f208%2c373 .

5.CONTINUATION,https://patents.google.com/patent/US20120072039A1/en?oq=US20120072039A1 .

6. CONTINUATION 9,395,707 B2, https://patents.google.com/patent/US9395707B2/en .

7. CONTINGENCY ANALYSIS TOOL FOR ELECTRIC DISTRIBUTION GRID MANAGEMENT, http://www.google.com/patents/US8583405 .

8. CAPITAL ASSET PLANNING SYSTEM, http://www.google.com/patents/US8725625 .

9. METRICS MONITORING AND FINANCIAL VALIDATION SYSTEM (M2FVS) FOR TRACKING PERFORMANCE FROM CAPITAL OPERATIONS, AND MAINTENANCE INVESTMENTS DURING SMART GRID MANAGEMENT OF ELECTRIC TRANSMISSION AND DISTRIBUTION, https://www.google.com/patents/US8725665?dq=8725665&hl=en&sa=X&ei=YIzJU4G8KIiSyASc-oCQBg&ved=0CB4Q6AEwAA .

10. MACHINE LEARNING FOR POWER GRIDS, https://www.google.com/patents/US8751421?dq=8751421&hl=en&sa=X&ei=pIzJU6m0KcqxyATf74HYCA&ved=0CB4Q6AEwAA .
11. SYSTEMS AND METHODS FOR MARTINGALE BOOSTING IN MACHINE LEARNING, http://www.google.com/patents?vid=8036996&printsec=overview .
12. INNERVATED STOCHASTIC CONTROLLER FOR REAL TIME BUSINESS DECISION-MAKING SUPPORT, http://www.google.com/patents?hl=en&lr=&vid=USPAT7395252&id=qDCrAAAAEBAJ&oi=fnd&dq=+%22ANDERSON,+ROGER+N%22&printsec=abstract#v=onepage&q=&f=false .
13. INNERVATED STOCHASTIC CONTROLLER FOR REAL TIME BUSINESS DECISION-MAKING SUPPORT, http://www.google.com/patents?hl=en&lr=&vid=USPAT7395252&id=qDCrAAAAEBAJ&oi=fnd&dq=+%22ANDERSON,+ROGER+N%22&printsec=abstract#v=onepage&q=&f=false .
14. METHOD FOR IDENTIFYING SUBSURFACE FLUID MIGRATIONAL PATHWAYS USING 3-D AND 4-D SEISMIC IMAGING, https://patents.google.com/patent/US5586082 .

AI/ML SOFTWARE PATENTS APPLIED FOR:

1. TOTAL PROPERTY OPTIMIZATION SYSTEM FOR ENERGY EFFICIENCY AND SMART BUILDINGS, https://docs.google.com/file/d/0B7Am-1xPqJfYckdjU2RMNVJzSkU/edit?pli=1 .
2. CONTROLLER FOR DISTRIBUTED ELECTRICAL ENERGY STORAGE MANAGEMENT, https://patents.google.com/patent/US20130158725 .
3. ADAPTIVE STOCHASTIC CONTROL FOR DYNAMIC TREATMENT OF CYBER-PHYSICAL SYSTEMS, https://www.google.com/patents/WO2013023178A1?cl=en&dq=PCT/US12/050439&hl=en&sa=X&ei=cxZgUuzxO5H64AOe4IAQ&ved=0CDkQ6AEwAA .
4. ADAPTIVE STOCHASTIC CONTROLLER FOR DISTRIBUTED ELECTRICAL ENERGY STORAGE MANAGEMENT, http://www.google.com/patents/WO2011106519A1?cl=en .
5. ADAPTIVE STOCHASTIC CONTROLLER FOR ENERGY EFFICIENCY AND SMART BUILDINGS, https://docs.google.com/file/d/0B7Am-1xPqJfYQnNJQnAyRTBHMFk/edit?pli=1 .
6. ADAPTIVE STOCHASTIC CONTROL FOR LOAD AND SOURCE CONTROL, https://docs.google.com/file/d/0B7Am-1xPqJfYcWkzVTFwR1lCcWM/edit?usp=sharing&pli=1 .

Geopolymers & Hybrid Inorganic Polymers for Ambient Temperature Synthesis

by Waltraud M. Kriven, Member EUAS

Short Biography

(a) Name, Organization and Contact Information:
Prof. Waltraud M. Kriven
Department of Materials Science and Engineering,
University of Illinois at Urbana-Champaign

(b) Professional Preparation

B.Sc.	*Physical and Inorganic Chemistry*	*Univ. of Adelaide, South Australia*	*1970*
B.Sc. (Hons)	*Physical and Inorganic Chemistry*	*Univ. of Adelaide, South Australia*	*1971*
Ph.D.	*Physical and Inorganic Chemistry*	*Univ. of Adelaide, South Australia*	*1976*

Sept. 1976 – April 1977 *Post-doctoral teaching and research fellow, University of Western Ontario, London, Ontario, Canada*

April 1977 – May 1980 *Post-doctoral researcher and Lecturer, Lawrence Berkeley Laboratory, and the Department of Materials Science and Mineral Engineering, University of California, Berkeley, respectively.*

May 1980 – Nov 1983 *Visiting research scientist, high voltage electron microscopy, Max Planck Institute, Stuttgart, Germany*

Nov 1983 – Feb 1984 *Post-doctoral researcher, Department of Materials Science and Mineral Engineering, University of California, Berkeley*

(c) Appointments

1995 – present *Full Professor, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign*

2007 -2012 *Affiliate Professor, Department of Bioengineering*

2009 – present *Affiliate Professor, Department of Mechanical Science and Engineering*

1987 – 1995 *Associate Professor, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign*

Feb 1984 – 1987 *Visiting Research Associate Professor, Department of Ceramic Engineering, University of Illinois at Urbana-Champaign*

(d) 303 research publications, 57 conference proceedings, 27 books, edited or co-edited, 39 plenary and keynote talks, 257 invited talks, 472 conference talks, 5 patents, 6th is pending

In the area of geopolymers, Kriven has written over 70 research papers and co-edited 21 conference proceedings which were published by the American Ceramic Society, as Ceramic Transactions (Vols. 153, 165, 175, 244) and Ceramic Engineering and Science Proceedings (Vols 26 - 40). During the past 5 years Kriven has been a symposium co-organizer on 3-4 international conferences on geopolymers per year.

(e) Research areas:

- *Geopolymers and hybrid inorganic polymers for ambient temperature synthesis*
- *Synthesis of oxide ceramic powders by the organic steric entrapment method*
- *Microstructure characterization by scanning and transmission by electron microscopy (SEM, TEM, EDS, HVEM, HREM, XPS)*
- *In situ, in air high temperature (2000°C) synchrotron XRD and Rietveld studies*

- *Structural ceramic composites and oxide fibers*
  (design, fabrication, characterization and mechanical evaluation)

(f) Professional Affiliations:

Academician, World Academy of Ceramics (2004)
Member, European Union Academy of Sciences (2020)
Fellow of the American Ceramic Society (1995)
Fellow of the Australian Ceramic Society (2009)

What are geopolymers? – Introduction

Geopolymers are inorganic poly silicate-aluminate polymers or chemically bonded ceramics centered around the nominal formula $M_2O•Al_2O_3•4SiO_2•11H_2O$ where M = group I element and the amount of water is variable, depending on the particle size and specific surface area of the aluminosilicate starting material. They are refractory, inorganic polymers formed from both aluminum and silicon sources containing AlO_4^- and SiO_4 tetrahedral units, under highly alkaline conditions (NaOH, KOH, CsOH) at ambient temperatures. Therefore they are a rigid, hydrated, alumino-silicate solid containing group I, charge-balancing cations which result in an amorphous, cross-linked, impervious, acid-resistant, 3-D structure.

The term "geopolymer" has different meanings to different scientific communities. In materials science geopolymers are made from kaolinite clay of composition $Al_2O_3•2SiO_2•2H_2O$ which was heated at ~750°C/2 hours and converted to amorphous metakaolin ($Al_2O_3•2SiO_2$). When mixed under high shear with water glass solution (e.g. of composition $M_2O•2SiO_2•11H_2O$), it undergoes dissolution, polycondensation and precipitation to form a geopolymer solid where all the silicate and aluminate tetrahedral are corner shared.[1-8]

In the civil engineering community the term "geopolymers" refer to the product resulting from high shear mixing of class F fly ash mixed with ground granulated blast furnace slag waste products. The solid is also amorphous or crystalline but it is based on the calcium silicate hydrate (CSH), C(A)SH, KASH, NASH) (i.e. charge balanced with Na^+ or K^+ ions) binder phases which form cements. In this structure, the silicate or aluminate tetrahedra form layers sharing only two or sometimes three corners, and are separated by layers of $Ca(OH)_2$. CSH is the main binder phase in Portland cement. [9-11] One main difference between the cements versus geopolymers is that geopolymers are chemically stable up to 1,000°C, after which they crystallize into ceramic.

When composites are formed with metakaolin-based geopolymers, some mechanical strength can be still be retained. Cements, on the other hand, contain significantly more water and so steadily decompose with increasing temperature, losing their mechanical strength. Thus metakaolin-based geopolymers are made like a cement but can behave like a ceramic, while cements will always remain as low temperature capable cements (Fig. 1). The difference between molecular structures of alkali activated cements versus geopolymers is illustrated in Figs. 2 and 3 below.

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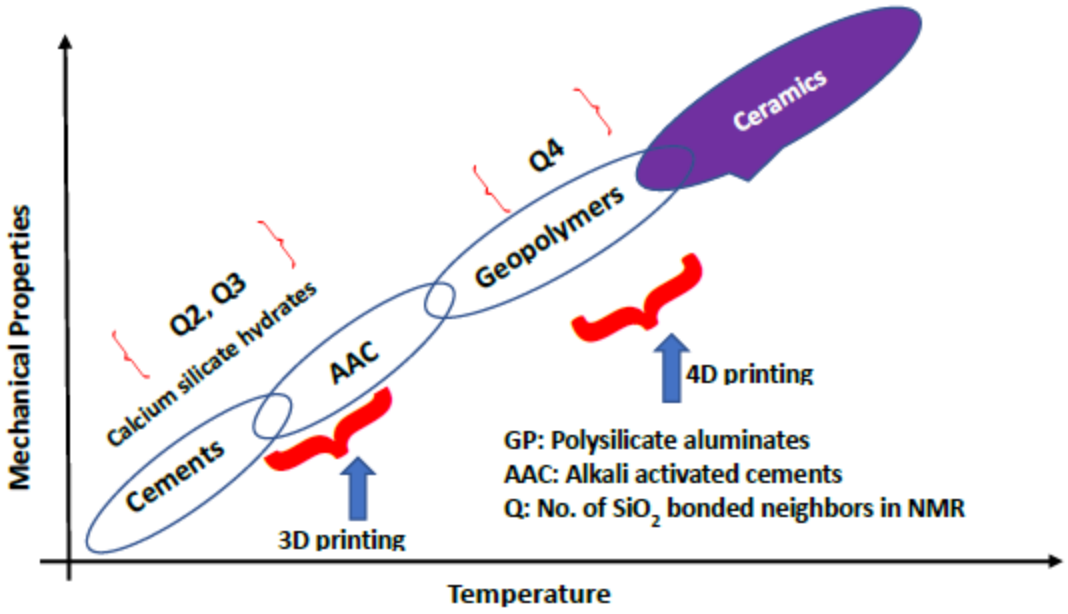

Fig. 1. Schematic diagram of the relationship between metakaolin-based geopolymers and waste material, class F fly ash and slag-based geopolymers.

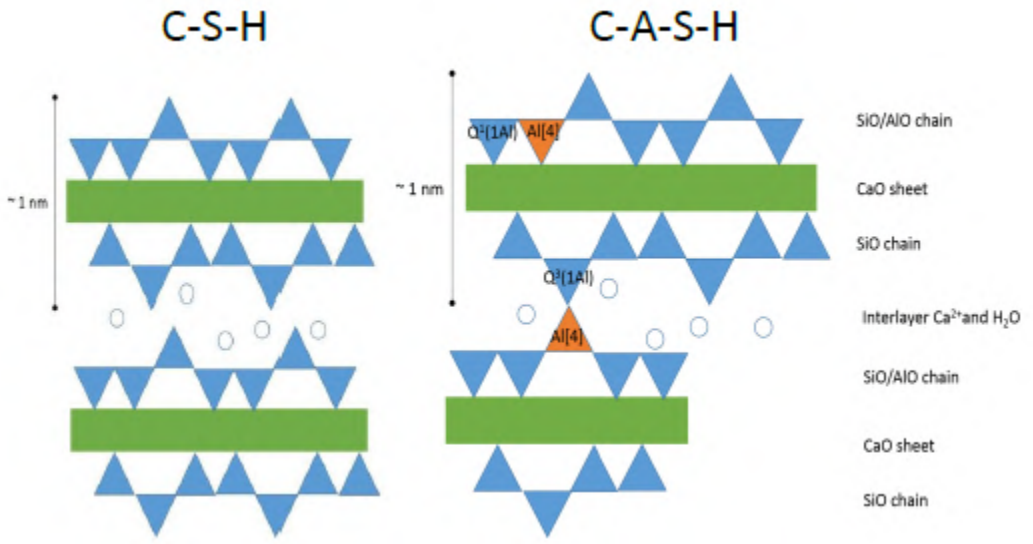

Fig. 2. Molecular structure of C-S-H and CASH cements. Tetrahedra share only 2 or 3 corners (Q2, Q3).[9-11]

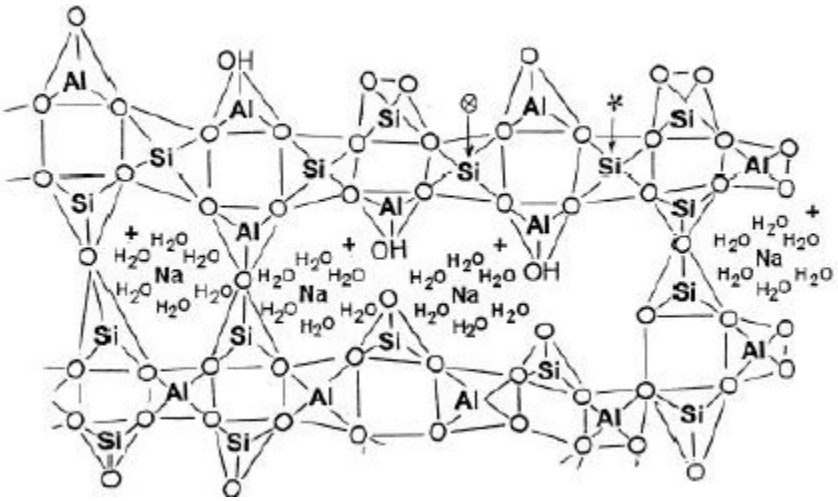

Fig. 3. Molecular structure of sodium-based geopolymer where all tetrahedra share 4 corners (Q4).[4,5]

The Long Pathway from Immunology to Stem Cells

by Carlos Martínez, Member EUAS

Short Biography

Professor of Immunology, Natl Center of Biotechnology, Spanish National Research Council (CSIC) . Madrid, Spain

Positions

- Assistant Professor in Immunology, Dept of Immunology, Clínica Puerta de Hierro, Madrid, 1979
- Member, Basel Institute for Immunology, Basel, 1979-1981
- Associate Professor, Dept of Immunology, Univ. of Umeå, Sweden, 1981
- Charge de Recherche, Centre National de la Recherche Scientifique (CNRS), Paris, France, 1982-1983
- Professor of Immunology, National Research Council and Centro de Biología Molecular, Univ. Autónoma, Madrid, Spain, 1986-1993
- Visiting Professor, Max Planck Institute for Immunology, Freiburg, Germany, 1987
- Visiting Scientist, Ontario Cancer Institute, Toronto, Canada, 1988
- Visiting Associate, California Institute of Technology, Pasadena, California, USA, 1992-1993
- Head, Dept Immunology & Oncology, Centro Nacional de Biotecnología, 1993- 2004
- Group Leader, Dept of Immunology & Oncology, Centro Nacional de Biotecnología, 2009-present

Administrative activities

- Head, Immunology Unit, Centro de Biología Molecular, Natl Research Council and Univ. Autónoma, Madrid, Spain
- Head, Dept of Immunology and Oncology, Centro Nacional de Biotecnología, Madrid
- President, Spanish National Research Council (CSIC), 2004-2008
- Secretary of State for Science Research, Spain, 2008-2009

External committees, honors and distinctions

- Member, NATO Scientific Committee on Research Grants
- Member, Expert's Committee of the UE in Science and Development (1994-1998)
- Vice-President, Spanish Society of Medical Chemistry (1986-1988)
- President, European Molecular Biology Conference (EMBC) (1996-2000)
- Vice-President, European Molecular Biology Laboratory Council (1997-2002)
- Member, Review Committee of the Human Frontier Science Program Organization (2000-2003)
- Member, Governmental Body of European Biosci (2000-2004)
- Member, European Molecular Biology Organization Council (2001-2007)
- Member, Governing Council, European Science Foundation (2004-2008)
- Vice-President, European Heads of Research Organization (EUROHORCS) (2004-2006)
- Board member, Fundacion de la Salud, Hospital Príncipe de Asturias, Univ Alcalá de Henares, Madrid
- Panel Chair, European Research Council (2007)
- Panel Chair, Programme Synergy Networks of the ERC (2012-2014)
- Member and Founder, Royal Academy of Sciences and Technology Hassan II of Morocco
- Member, Scientific Advisory Board, Venetian Inst of Molecular Medicine, Padova, Italy
- Member, Board of Trustees, Universidad Politécnica de Madrid,Spain.
- Member, Board of Trustees, International University Menéndez Pelayo, Spain
- Doctor honoris causa, Universidad de Leon (2005) and Universidad de Alcalá de Henares (2006)
- President, Scientific Advisory Board, Inst de Investigacion Sanitaria del Hospital Universitario de Asturias (ISPA). Spain

- Member, Identification Committee for the Selection of the Scientific Council of the European Research Council (ERC)

Committees and scientific societies

- Founder member, Spanish Society for Immunology
- Founder member, Spanish Society for Medical Chemistry
- Founder member, Spanish Society of Biotechnology
- Member, IUIS Committee
- Member, Board of European Network of Immunological Institutes (ENII)
- Member, European Molecular Biology Organization (EMBO)
- Member, European Cytokine Network Society
- Member, European Cell Death Organization (ECDO)
- Member, Iberoamerican Molecular Biology Organization (IMBO)
- Member, European Academiae
- Founder member, European Academy of Tumor Immunology
- Founder member, European Academy of Tumor Immunology

Awards

- Award, Royal Society of Natural Sciences, Spain 1990
- Award, Fundación Ciencias de la Salud, Spain 2000
- XI DuPont Prize for Science, Spain 2001
- VIII Premio Carmen y Severo Ochoa, Spain 2001
- Rey Jaime I Award for Scientific Research, Spain 2003
- Lilly Award for Preclinical Research, Spain 2004
- Award for Scientific Research, Castilla y León 2004
- International Galen Award for Scientific Research
- Gran Cruz de la Orden del Mérito Civil, 2012
- National Award for Medicine "Gregorio Marañón" , Spain 2010
- International Award of the Mexican Government for Science and Technology , Mexico, 2014

Trained as an immunologist my research focuses on immunology, cell and molecular biology, and stem cells, with emphasis on:

Selection of immune repertoire, lymphocyte activation and differentiation and its implication in autoimmune disease. This work, begun in the late 1970s, aimed to understand the mechanism of B lymphocyte activation by T cells, a key question in the immunology of the 1980s. I established a novel tissue culture technique to raise antigen-specific T cells to hapten-coated antigen-presenting cells. Successive *in vitro* stimulation allowed maintenance of helper T cell clones that trigger polyclonal B cells to antibody secretion when coated with the appropriate antigen or hapten (*Nature* 290:60, 1981; *Immunol Rev* 78:211, 1984).

I extended this initial interest in B cell activation to T lymphocyte activation, for which I worked out the mechanisms involved in mitosis and their consequences in triggering autoimmune disease. I thus contributed to characterizing the role of the forkhead transcription factor in T cell proliferation, and to understanding the relevance of decontrolled T cell proliferation triggered by lack of p21, which leads to memory T cell accumulation, autoantibody production, and development of lupus erythematosus. Finally, I addressed the role of the cohesin complex in mitosis regulation (*Nature* 413:744, 2001; *Nat Cell Biol* 3:761, 2001; *Nat Med* 6:171, 2000).

At this time, I was puzzled by one of the most cryptic enigmas in immunology at a time when it was thought that T and B cells shared clonally distributed receptors, the immunoglobulins. I found that immunoglobulin idiotype expression by T cells is not the result of receptor sharing, but a T cell selection process in the context of B cells; a series of experiments in mice lacking B cells showed that idiotype sharing by B and T cells was missing. These studies were extended to identify the relevance of the selection process

imposed by B cells on the T cell repertoire acquired during the first three weeks of development in mice, the implications of this selection for antibody responses, and its significance for vaccination (*Proc Natl Acad Sci USA* 81:4520, 1984; *Nature* 317:721, 1985; *Ann Rev Immunol* 7:209, 1989). We also showed the importance of telomere maintenance for antibody-mediated immune responses, supporting the idea that telomere elongation detected in wild-type spleens after immunization is telomerase-mediated (*EMBO J* 19:472, 2000), as well as the role of APRIL in the induction and/or maintenance of T and B cell responses (*J Clin Invest* 109:1587, 2002).

Our work on T cell development identified a new T cell subset, the so-called double-negative T cells, as the intermediate population in T cell development, described possible pathways for the T cell precursor developmental program, and showed that this subpopulation can have effector functions (*Proc Natl Acad Sci USA* 82:6268, 1985; *Proc Natl Acad Sci USA* 83:6985, 1986; *J Exp Med* 172:439, 1990). We identified the role of interleukin-2 in T cell development, showing that in man, double-negative T cell precursors express the intermediate affinity receptor for IL-2 and differentiate into effector g/d T cells in the presence of this cytokine. This differentiation pathway has physiopathological implications, since lack of IL-2 during this developmental stage triggers autoimmune disease. Correct administration of IL-2 through recombinant vaccinia virus bearing IL-2 prevents autoimmune disease, possibly by activating regulatory T cells or eliminating pathological cells (*Nature* 342:82, 1989; *Nature* 346:271, 1990).

This opened up an important area in the immunology of the 1990s, that of the cell lineage subpopulation involved in T cell development. We helped to identify a possible mechanism to generate T cells from T cell precursors, and to show that T cells with cytotoxic activity can also express the CD4 coreceptor molecule (*J Exp Med* 168:2231, 1988; *J Exp Med* 177:19, 1993).

Chemokines in leukocyte migration and infection. My lab identified one of the pathways involved in chemokine-triggered signaling, which involves dimerization of GPCR family receptors to activate a downstream JAK/STAT pathway. This was the first demonstration that this receptor family activates a pathway shared with the cytokines, that of receptor dimerization and activation of a tyrosine kinase pathway. This remarkable finding allowed identification of crossregulation between the cytokine and the chemokine responses. Chemokine receptor dimerization has far-reaching implications for the prevention of HIV-1 infection, (*Nature* 400: 7272, 1999). In addition to generating basic knowledge for biomedicine, my studies allowed testing of a strategy based on new biotechnological tools for asthma treatment. In this work with chemokines, we showed that blocking CCR2 in animal models prevents asthma (*Proc Natl Acad Sci USA* 96:3628, 1999; *Nature* 400: 273, 1999; *Proc Natl Acad Sci USA* 97:3308, 2000; *EMBO J* 20:2497, 2001; *Ann Rev Immunol* 19:3971, 2001; *Nat Immunol* 5:216, 2004).

We helped identify the role of the leukocyte polarization necessary for cell migration in chemotactic responses. I showed that, in T cells, this process involves migration of chemokine receptors to the leading cell edge and of adhesion molecules to the uropod at the rear of the cell; other cell lineages only express the leading edge during the polarization step. The proteins at both cell poles are incorporated and transported in membrane raft microdomains that contain GM1 at the uropod and GM3 at the leading edge (*J Exp Med* 186:153, 1997; *EMBO J* 18:6211, 1999; *Proc Natl Acad Sci USA* 98:9642, 2001, *Nat Rev Immunol* 3:557, 2003).

Cancer and development. My laboratory contributed to current understanding of the mechanisms that activate the apoptotic program by identifying a new gene (*DIO-1*) that displays transcriptional activity, as well as a new structural motif homologous to BH3, the so-called GH3. This was determined using *DIO-1* in Drosophila, and further demonstrating that it also triggers apoptosis in mammals. We identified the role of transcription factors such as Aiolos, also involved in lymphocyte development, and that of calpastatin in B cell apoptosis (*EMBO J* 18:3419, 1999; *Proc Natl Acad Sci USA* 96:7992, 1999; *EMBO J* 18:4988, 1999, *EMBO J* 21:3327, 2002; *Nat Rev Immunol* 3:557, 2003).

We also studied the role of APRIL in the disorganization of mesenteric lymph nodes and Peyer's patches, and the development of progressive hyperplasia in lymphoid tissues, with cell infiltration into nonlymphoid tissues such as kidney and liver. Moreover, we found significantly increased APRIL levels in sera of B cell chronic lymphoid leukemia (B-CLL) patients, indicating that APRIL promotes onset of B-1-associated neoplasms and that APRIL antagonism might provide a therapeutic strategy to treat B-CLL patients (*Cancer Cell* 6:399, 2004). We also contributed to the identification of the mechanisms involved in limb development using chick and mouse models, in which we showed the critical role of the *Meis-1* and *Meis-2* genes for limb development, as well as in lymphoma development. Our studies indicate that this gene family might also be implicated in control of hematopoiesis (*Nature* 394:196, 1998; *Nature* 402:425, 1999).

Stem cell renewal and differentiation. Recently I have centered on identifying of the mechanisms involved in the control of stem cell self-renewal and differentiation. I have identified Dido (*Proc Natl Acad Sci USA* 96:7992, 1999) as a stemness marker and a locus involved in ESC differentiation. The *Dido* gene complex encodes three splice variants, Dido1 (the smallest), Dido2 and Dido3. All attempts to date to delete Dido, in *in vitro* cell lines or in mice, show that this deletion is incompatible with life. N-terminal truncation of *Dido* (Dido□Nt) *in vivo* provokes aneuploidy, centrosome amplification, and increased incidence of hematological myeloid neoplasms. Alterations in Dido are associated to myelodysplastic syndrome (MDS) in humans. C-terminal truncation of *Dido3* (Dido□Ct) *in vivo* results in embryonic death at day 7.5-8 dpc, and stem cells derived from Dido□Ct mutants do not differentiate, yet retain their self-renewal capacity (*Cell Rep* 4 :4148, 2013, *J Clin Invest* **115**:2351, 2005). We also identified a synthetic phenotype in Dido□Nt/□Ct double heterozygotes that drives severe perinatal lethality, and thus identifies an important role for the *Dido* gene in craniofacial development. The few Dido□Nt/□Ct mice that reached adulthood had alterations in metabolism, cilia, and neuromuscular development that highlight Dido involvement in many physiological functions, including behavioral abnormalities and metabolic syndromes (*Proc Natl Acad Sci USA 112:4803, 2015*). We identified a role for Dido3 in delivery of actin-dependent histone deacetylase 6 (HDAC6) to the primary cilium (*Nat Commun* 5:3500, 2013).

Targeting the murine *Dido* gene causes merotelic attachments, centromere distortion, and lagging anaphase chromosomes (*Proc Natl Acad Sci USA 104:2691, 2007, Proc Natl Acad Sci USA 107:4159, 2010).* Like Mad2-/-p53-/- fibroblasts and nocodazole-blocked cells, *Dido* mutant cells accumulate double strand DNA breaks (DSB) during mitosis. Breaks generated by spindle defects localize on or adjacent to centromeres, although overall DSB repair defects can be excluded in the *Dido* mutant, and centromeric DSB are repaired as efficiently as elsewhere in the chromosome. In accordance with the current view of merotelic attachments, breaks appear to affect only one of the two sister chromatids.

Directed Evolution of Selective Enzymes as Catalysts in Organic Chemistry and Biotechnology

by Manfred T. Reetz, Member EUAS

Short Biography

Manfred T. Reetz (born on August 13th 1943 in Hirschberg, Germany) is an internationally renowned German synthetic organic chemist. He obtained the Master degree in Chemistry (University of Michigan/USA, 1967) and the doctoral degree in 1969 under the direction of Ulrich Schöllkopf at Göttingen University/Germany (1969). He started independent work at Marburg University, and then accepted the appointment at Bonn University as Associate Professor, before becoming Full Professor of organic chemistry back in Marburg (1980-1991), where he focused on organometallic chemistry and novel synthetic methods. Thereafter, Manfred Reetz moved to the Max-Planck-Institut für Kohlenforschung in Mülheim/Germany as successor to Günther Wilke, where he served as Managing Director from 1993 to 2002. During this time he initiated new research projects, especially the concept of directed evolution of selective enzymes as catalysts in organic chemistry and biotechnology, and also restructured the institute with the creation of five Departments, each headed by a respective Director. Following formal retirement as Director in 2011 at age 68, he became the first Hans-Meerwein-Research-Professor in the Chemistry Department of Marburg University. In 2019 he returned to the MPI in Mülheim, and also accepted the position of a Professor of the "Reetz Laboratory" in China at the Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences (TIB-CAS). Over the years, Reetz has had numerous administrative jobs, including chairman of the Chemistry Department of Marburg University, Senator of the German National Academy of Sciences Leopoldina, member of the Ethics Council of the Max-Planck-Society, of the Editorial Board of Angew. Chem, and of the Kuratorium of the Krupp-Foundation. For a complete list, see his website at kofo.mpg.de/en/research/biocatalysis.

Reetz has received numerous prestigious national and international prizes and awards, including Otto Hahn Prize (Germany), Karl Ziegler Prize (Germany), Otto Bayer Prize (Germany), Prelog Medal (Switzerland), Arthur C. Cope Award (USA), IKCOC Award (Japan), Yamada-Koga Prize (Japan), Distinguished Scientist of the Chinese Academy of Sciences (China), and the Tetrahedron Prize for Creativity in Organic Chemistry (international). For a complete list, see the Reetz website. He is also a member of the German National Academy of Sciences Leopoldina and of the Royal Netherlands Academy of Arts and Sciences. His papers and reviews are highly cited, the h-factor in mid 2020 reaching a value of 118 (Google) with more than 53,000 citations.

As Manfred T. Reetz noted in his 2020 review article,[1] the most important, innovative and indeed seminal contribution in his scientific career was the suggestion and extensive experimental implementation of the concept of directed evolution of stereoselective enzymes. When the Reetz group started this project in 1994-1995, it was a scientific adventure and a notable financial risk. Enzyme

directed evolution is a protein engineering method which had been used only for enhancing protein stability, as the groups of R. Hageman (1986), J. A. Wells (1985) and F. H. Arnold (1993) had reported. However, this was of little interest to organic chemists, because it was well known that stability can also be achieved by enzyme immobilization. In contrast, stereoselectivity stands at the heart of organic chemistry, since very many pharmaceuticals, plant-protecting compounds, fragrances and natural products are chiral. The new concept for producing stereoselective catalysts is quite different from the usual procedure applied in the development of man-made chiral transition metal complexes or organocatalysts. In repeating cycles comprising mutagenesis, protein expression, colony harvesting and screening for stereoselectivity, evolutionary pressure is built up as schematized in Figure 1.[1,2].

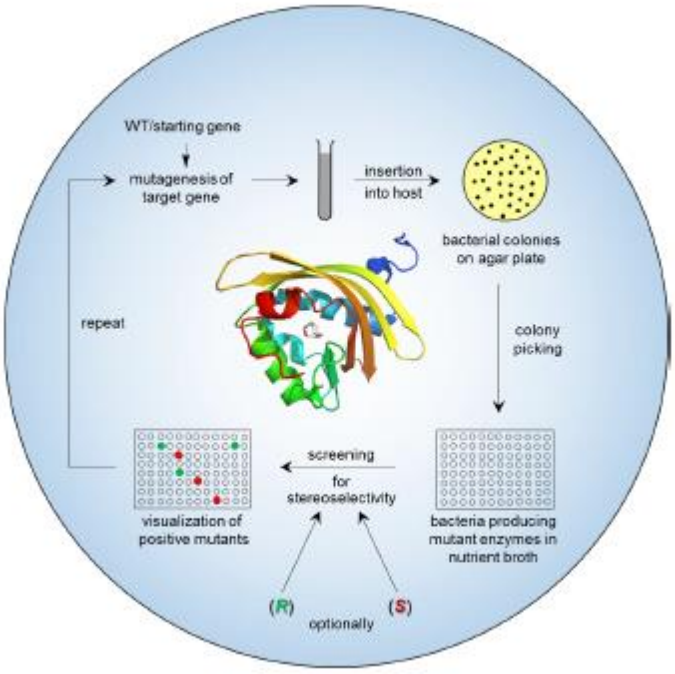

Fig. 1. Concept of directed evolution of stereoselective enzymes as catalysts in organic chemistry and biotechnology.[1,2]

Proof-of-principle was first demonstrated in 1997,[2] the kinetic resolution of the racemic ester *rac*-**1**, catalyzed by the lipase from *Pseudomonas aeruginosa* (PAL) serving as the model system (see below). In four cycles involving error-prone polymerase chain reaction (epPCR), the selectivity factor *E*, reflecting the relative rates of reaction of the two enantiomers, rose from 1.1 to 11.3 in favor of the *S*-substrate (Figure 2). At the time, this unique breakthrough was celebrated extensively in the Reetz group! Subsequently the same procedure was applied for reversing enantioselectivity in favor of the *R*-substrate.

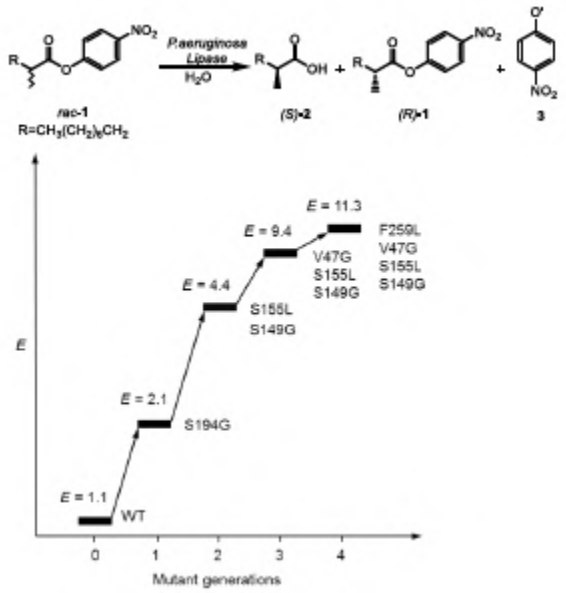

Fig. 2. First example of directed evolution of a stereoselective enzyme, in this case the lipase PAL, as catalyst in the hydrolytic kinetic resolution of *rac*-**1**.[2]

Since a selectivity factor of E=11.3 does not suffice for real (industrial) applications, and the benefit of the 5th cycle was only modest, the Reetz group initiated long-term methodology development based on other molecular biological mutagenesis methods. This included focused saturation mutagenesis at the binding pocket of enzymes, DNA shuffling (Stemmer technique) and combinations thereof.[3] By 2004, the concept was clearly established, and other groups had joined efforts in generalizing the concept using other enzyme types.[4] In 2005-2007, the Reetz group continued to focus on saturation mutagenesis with the development of the systematic Combinatorial Active-site Saturation Test (CAST) and Iterative Saturation Mutagenesis (ISM)[5] for changing the shape of enzyme binding pockets (Figure 3), summarized in a monograph[6] and once again in the 2020 review.[1] These crucial developments for reshaping the binding pocket of enzymes correspond to Emil Fischer's famous lock-and-key hypothesis postulated more than 100 years ago!

First generation CAST/ISM approach to directed evolution was used by many academic and industrial groups for the catalytic formation of chiral compounds, especially in the pharmaceutical industry. The refined second generation CAST/ISM technique is even more efficient and widely employed, including vaccine production and potential universal blood production, reviewed in 2020.[1]

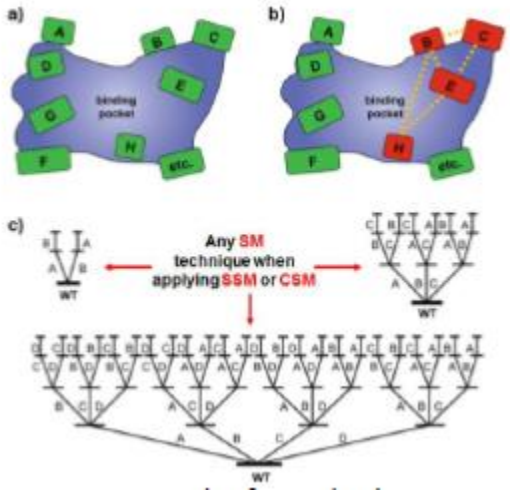

Fig. 3. Strategies for re-shaping an enzyme's binding pocket.[1,5,6]

Learning lessons concerning the intricacies of enzyme mechanisms via directed evolution was also a central issue in the Reetz group to the present day.[7,8] Most recently, machine learning techniques were likewise applied in the quest to make directed evolution of selectivity more efficient.[1] In addition to lipases, other enzyme types for different kinds of chemical transformations were successfully tested, including reductases for the enantioselective reduction of ketones and cytochrome P450 monooxygenases for regio- and stereoselective hydroxylation of steroids and other substrates leading to products of high pharmaceutical value. The idea of directed evolution of artificial metalloenzymes for promiscuous reactions, first announced by Reetz in 2000-2002, is also a standard procedure today.[9]

Today numerous groups utilize the approaches and techniques introduced by Manfred T. Reetz during the last 25 years. These developments have contributed heavily to making enzyme catalysis generally attractive and useful for a sustainable as well as ecologically and economically viable chemistry.

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The Self-Cleansing Capacity of Aquatic Systems (Oceans, Rivers, Lakes, Groundwater)

by Peter H. Santschi, Member EUAS

Short Biography

Dr. Peter H. Santschi is a Regents Professor of Oceanography and Marine Sciences at the Texas A&M University, Galveston, TX, USA. He received his training in Geochemistry and Oceanography during his post-graduate work at L-DEO of Columbia University, N.Y., after graduating from the University of Bern, Switzerland, with a Ph.D. in Chemistry. Santschi's research interests include Marine Chemistry, Environmental Chemistry and Environmental Radiochemistry; trace element interactions with natural organic matter; tracer applications in natural water systems using stable and radioactive isotopes. Since 2000, he is associate editor of the journal Marine Chemistry. He is an author or co-author of 370+ journal articles and 45 book chapters on these subjects, which, over the years, have received more than 23,000 citations. His google impact factor h is 85. More on his research can be found at http://loer.tamug.edu/people/Santschi/index.html, and https://scholar.google.com/citations?user=ZKGyOTsAAAAJ&hl=en&oi=ao.

Peter H. Santschi received **numerous national and international awards**, e.g., he was elected Member of the European Union Academy of Sciences (EUAS) (2020), Geochemical Fellow of the Geochemical Society and the European Association of Geochemistry (2017); Fellow of the American Geophysical Union (2014), which are given annually to only 0.1% of the 60,000 members; received the Distinguished Achievement Awards in Graduate Student Mentoring (2013) from Texas A&M's Association of Former Students; Regents Professor of Texas A&M University (2009), and received the Association of Former Student Distinguished Achievement Award for Research from Texas A&M University (2004). These awards were not possible without testimony by many prestigious international researchers.

He is a member of many Academic Advisory or Review Panels, as well as a Visiting Professor at national and international Universities, e.g., at Lamont-Doherty Earth Observatory of Columbia University (1982-1988), University of Rhode Island, School of Oceanography (1986), Dept. of Geology and Dept. of Chemistry, University of Geneva, Geneva, Switzerland (1996), Dept. of Chemistry and Biochemistry, University of Bern, Bern, Switzerland (2002), Dept. of Chemistry, University of Geneva, Geneva, Switzerland (2003), Swiss Institute of Technology, ETH, Zurich, Switzerland (2003), National Taiwan University, Taipei, Taiwan (2003), and Hong Kong University of Science and Technology

(2004), National Center for Oceanographic Research, NCOR (2008).

Summary of accomplishments in Environmental Science related to improving our understanding of the self-cleansing capacity of natural aquatic systems

During his 45-plus year career in environmental science, Santschi has gained and communicated novel insights into some of the blueprints of the aquatic environment, spanning from rain water, rivers and lakes to groundwater, from surface to deep ocean. During his long research career, he, together with 40+ graduate students, post-doctoral fellows and scientists all over the world, was able to pioneer new concepts and approaches that were truly **transformational**. The unifying theme of his research has been the **study of the self-cleansing capacity of natural aquatic systems**: in particular, the importance of natural organic matter compounds for particle, radionuclide, and trace element cycling in aquatic systems. The importance of natural organic matter was not obvious in aquatic chemistry, as for many decades, the dogma was that metal behavior is mostly controlled by inorganic ligand interactions. His research involves the main agents that can ameliorate impact (e.g., toxicity, mobility) of potential pollutants to aquatic biota, i.e., microbially produced macromolecular substances that occur in the colloidal phase. This phase is mostly composed of nano-sized exopolymeric substances, as well as terrestrially derived humic substances, both of which can, at times, greatly help to control the efficiency of the self-cleansing capacity of aquatic systems. Natural colloids in aquatic systems are thus, to a large extent, derived from biological production and degradation of natural particles. Therefore, Santschi's main contributions and impacts in environmental geochemistry are on the role of macromolecular natural organic matter on engineered nanoparticle, trace metal, and radionuclide speciation, transport, and cycling.

Dr. Santschi's **seminal contributions** to science, more specifically to the field of environmental biogeochemistry and radiochemistry, have thus included major **transformational** breakthroughs, e.g., the Colloidal (or Brownian) Pumping Concept that led to paradigm shifts in aquatic science (see below), and sustained impact, with his most cited papers providing unifying chemical and physic-chemical concepts explain pollutant behavior in aquatic environments, including articles published from the 1980s, 1990s, and 2000s. This transformational "Colloidal or Brownian Pumping Model" was able to simulate observations of apparent particle concentration effects on both the widely observed particle-water distribution coefficients and the model kinetic constants of trace element and radionuclide uptake onto natural particles, given the observed colloidal fractions of trace metals and radionuclides. His work then stimulated many other researchers to build on these novel concepts. Over the years following this transformational work, he tackled the challenging question of macromolecular organic compounds that occur in the colloidal phase and act as carrier molecules for specific trace elements and radionuclides. Due to the numerous difficulties in finding such compounds at relevant but trace levels in the midst of thousands of other compounds, selective separation and purification chemistry had to be thoroughly investigated before state-of-the-art instrumentation could be applied.

Recent reviews of aquatic science subject areas

Santschi, P.H. 2018. Marine colloids, agents of the self-cleansing capacity of aquatic systems: Historical perspective and new discoveries. Marine Chemistry 207, 124–135. https://doi.org/10.1016/j.marchem.2018.11.003

Colloids in the ocean are mainly composed of natural organic matter (NOM), with trace amounts of metals, metalloids, radionuclides, pollutants, and variable amounts of anthropogenically produced engineered nanoparticles and nanoplastics. State-of-the-art sampling and instrumental techniques were required to unravel both size spectra and chemical composition.

Chemical components of colloidal macromolecular organic matter (COM) include aquagenic substances (composed of microbially produced Exopolymeric Substances (EPS), gels, transparent exopolymer particles (TEP) and TEP precursors), and pedogenic substances (mostly humic and fulvic matter). COM can be bioavailable and biodegradable. EPS in aquatic systems can form flocs of Marine Snow (MS) or Marine Oil Snow (MOS). EPS is thus important in initiating and maintaining aggregation, flocculation, and sedimentation processes of particles and microorganisms that act also as sorbents of pollutants, a process that contributes in a major way to the 'self-cleansing capacity' of aquatic systems.

COM contains a diverse array of functionalities which can make them good metal chelating agents, amphiphilic and surface-active pH-sensitive and redox-active. Due to numerous electrostatic and hydrophobic interactions between different moieties and ligand groups within a macromolecule, equilibrium constants, Ki, will become distribution functions for most reactions rather than fixed constants, as is common for low molecular weight organic molecules.

Colloidal pumping of trace substances bound to EPS and other reactive macromolecular NOM compounds is counteracting the prevailing pathway of degradation of the bulk macromolecular NOM. Due to strong sorption capabilities for stable and radioactive metal ions, particle- and colloid-reactive radionuclides are useful to trace particle and organic carbon fluxes in the ocean.

Open research questions include the role of different mechanisms that affect size spectra and composition of EPS in response to changing conditions, the role of macromolecular organic carrier molecules of radioactive and other trace substances that are used as oceanographic tracers; the potential use of the protein/carbohydrate ratio as a predictor of colloid or particle stickiness, aggregation or emulsification processes, and the importance of reactive oxygen species (ROS) mediated polymerization reactions of proteins and other molecules, which are part of EPS, for MS and MOS formation..

Santschi, P.H., Xu, C., Schwehr, A.K., Lin, P., Sun, L., Chin, W.-C., Kamalanathan, M., Quigg, A. 2020. Can the protein/carbohydrate (P/C) ratio of exopolymeric substances (EPS) be used as a proxy for its 'stickiness' and other biophysical properties? Perspective article in Marine Chemistry, https://doi.org/10.1016/j.marchem.2019.103734.

Microbially secreted exopolymeric substances (EPS), rich in polysaccharides and proteins, make up an important part of natural organic matter in the ocean, especially marine snow. While the attention in most previous oceanographic literature focused on the

role of polysaccharides in EPS functions, less is known about the role of proteins, especially the protein/carbohydrate (P/C) ratio of particles and colloids (macromolecular fraction), in marine systems. EPS associated with particles forms a biofilm, whereby proteins are not only involved in cell surface attachment, but also in the stabilization of the biofilm matrix, and the development of a three-dimensional biofilm architecture**.** Here, we provide a perspective based on the most recent literature on EPS, marine oil spills and waste water treatment to describe the relationship between the P/C ratio of EPS and a number of biophysical properties related to biopolymer aggregation (e.g., relative hydrophobicity, surface activity and surface tension, attachment efficiency, light-induced chemical crosslinking), and the sedimentation efficiency of marine snow in marine environments.

Yeager, C.M., Amachi, S., Grandbois, R., Kaplan, D.I., Xu, C., Schwehr, K.A., and Santschi, P.H. 2017. Microbial transformation of iodine: From radioisotopes to iodine deficiency. Advances in Applied Microbiology, 101, 83-136. https://doi.org/10.1016/bs.aambs.2017.07.002

Iodine is a biophilic element that is important for human health, both as an essential component of several thyroid hormones, and on the other hand, as a potential carcinogen in the form of radioiodine generated by anthropogenic nuclear activity. Iodine exists in multiple oxidation states (-1, 0, +1, +3, +5 and +7), primarily as molecular iodine (I_2), iodide (I^-), iodate (IO_3^-) or organic iodine (org-I). The mobility of iodine in the environment is dependent upon its speciation and a series of redox, complexation, sorption, precipitation and microbial reactions. Over the last 15 years, there have been significant advances in iodine biogeochemistry, largely spurred by renewed interest in the fate of radioiodine in the environment. We review the biogeochemistry of iodine, with particular emphasis on the microbial processes responsible for volatilization, accumulation, oxidation and reduction of iodine, as well as the exciting technological potential of these fascinating microorganisms and enzymes.

C4. Verdugo, P., Santschi, P.H. 2010. Polymer dynamics of DOC networks and gel formation in seawater. Deep Sea Research II, 57, 1486-1493. https://doi.org/10.1016/j.dsr2.2010.03.002

The ocean plays a major role in global biogeochemical carbon cycling; it holds an important reservoir of reduced organic carbon, mostly in the form of dissolved organic carbon (DOC), and processes about one-half of the total primary production of the planet. Dissolved molecules present between living and assimilable size extremes ($\sim$1000 nm^{-1} nm), constitute the most abundant form of remnant biochemicals in the ocean, outweighing the total living biomass by a factor of roughly 200. Because DOC is the fundamental substrate for marine microorganisms, and is primarily composed by small refractory biopolymers, this prompted the idea that the ocean might function as a huge repository of recalcitrant carbon. The missing link that elucidates this paradox and explains how the rich and vast stock of DOC becomes available to bacteria was the discovery that DOC throughout the water column remains in reversible assembly/dispersion equilibrium forming porous microscopic gels (Chin et al., Nature 391, 568-572, 1998). This abiotic DOC-POM shunt yields a microgel pool containing $\sim$70 gigatons of carbon forming discrete patches of high nutrient concentration that can be readily colonized by microorganisms. The presence of this huge gel mass in seawater extending far into the dark

ocean has ramifications that might well scale nonlinearly through the microbial loop to the World Ocean and global climate system and it is fundamentally changing how oceanographers think about processes linking the microbial loop and biological pump to the rest of the biosphere and the geosphere. Even if a small fraction of DOC remains self-assembled, marine scientists will have to revise the rationale of established aquatic paradigms ranging from trace metal chelation, size–reactivity relationships, the microbial loop, the biological pump, colloid pumping, and humification. A ubiquitous, reversible DOC assembly/dispersion process implies a dynamic "patchiness" spanning from the molecular to the micron scale, where the assignment of static bulk features including dimension, concentration, functionalities and vertical fluxes can be open to question. This brief revision illustrates two case studies that show how simple methods and principles of polymer networks theory can be used to advance the understanding of one of the most intriguing and significant processes taking place in the ocean. Namely, the kinetics and thermodynamics of: (a) Ca-driven DOC self-assembly, and (b) hydrophobic bond-driven self assembly of DOC by amphiphilic exopolymers released by marine bacteria.

New 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 James I. Mueller Award from the American Ceramic Society (2020); 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 570 journal articles, 118 peer-reviewed conference papers, and 13 book chapters. Based on the Web of Science, his publications have over 20,300 citations, with an h-index of 71; based on Goggle Scholar, his publications have been cited over 27,700 times, with an h-index of 82.

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.

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, including nuclear power, space exploration, national security and ion-beam processing of nanostructures and opto-electronic devices. We have investigated the coupling between electronic and nuclear energy dissipation in single crystal 4H-SiC irradiated at 300 K with O, C, Si, Ti, and Ni ions over a range of energies, with the accumulation or irradiation damage characterized using Rutherford backscattering spectroscopy in channeling geometry. The damage production rate from nuclear energy loss (S_n) is observed to decrease with increasing electronic energy loss (S_e) of the incident ions. A dynamic threshold ($S_{e,th}$) in electronic energy loss is determined for each ion species, which defines two regions: i) $S_e > S_{e,th}$, where electronic energy dissipation fully suppresses damage production due to nuclear energy loss along incident ion paths, and ii) $S_e < S_{e,th}$, where simultaneous damage recovery due to S_e competes with damage production processes. The electronic energy loss threshold ($S_{e,th}$) increases sublinearly with incident ion atomic number. The assessment of $S_{e,th}$ and how it affects damage accumulation is important to advance the understanding of complex processes occurring under ion-solid interactions, as well as in the design of functional materials for opto-electronics and novel structural materials and devices tolerant to harsh thermal and radiation environments.

We have also investigated the effects of the electronic energy loss on defect production due to ion irradiation of silicon carbide using molecular dynamics simulations. Both 20 keV and 30 keV Si and C collision cascades were simulated, with and without the electronic energy loss. As expected, the results show fewer defects are produced when the electronic energy loss is accounted for in the simulations as a friction force. When the electronic energy loss is considered for C cascades, larger cluster sizes are formed; while in the case of Si cascades, there is a tendency for more smaller clusters when electronic energy loss is considered. In general, the simulations reveal that the role of electronic energy loss is more profound in the case of C ions, where the ratio of the electronic energy loss S_e to the nuclear energy loss S_n is much larger compared to the ratio for Si ions. These findings indicate that the ratio of S_e to S_n plays a critical role in the effects of the electronic energy loss on the response of SiC to ion irradiation.

We have investigated the formation of polar phonon modes, associated with room temperature ferroelectricity, in $SrTiO_3$ single crystals irradiated with Ti ions. Quantitative strain analysis reveals that irradiation-induced out-of-plane strain drives the centrosymmetric cubic $SrTiO_3$ to a tetragonal-like structure in the maximum damaged

region. Energy transfer from ions to electrons during ion irradiation yields defects in $SrTiO_3$ that also plays an important role for the room temperature ferroelectricity. Different from thin film techniques, the ferroelectricity in the ion irradiated $SrTiO_3$ can occur for much larger thicknesses, depending on the incident ion energy.

We have investigated the energy dissipation and track formation due to ion irradiation in $SrTiO_3$ and $KTaO_3$. Using molecular dynamics simulations combined with the inelastic thermal spike model, we have simulated 21 MeV Ni ion irradiation in pristine and pre-damaged samples. The results have been validated against experimental measurements and demonstrate that the level of initial disorder affects the electron-phonon interactions and the energy dissipation to the atomic structure. Thus, while defects are often considered to be unwanted, they can be used to manipulate the response of materials to electronic energy loss. The results predict that ion track size increases linearly for low levels of initial disorder, while track size exhibits a tendency to saturate for higher levels of initial disorder. This work emphasizes the importance of combining modeling and experiments in order to advance the understanding and predictive modeling of material response under irradiation. Further investigation of the synergistic effects of the pre-existing disorder and the electronic energy dissipation is need in a wider range of materials and ions in order to understand the radiation damage processes that take place on such short time scales.

Select Publications Related to This Research

1. W. A. Hanson, M. K. Patel, M. L. Crespillo, Y. Zhang, and W. J. Weber, Influence of electronic vs nuclear energy loss in radiation damage of Ti_3SiC_2, *Acta Materialia* **161**: 302-310 (2018).
2. G. Velisa, E. Wendler, L.-L. Wang, Y. Zhang, and W. J. Weber, Ion mass dependence of irradiation-induced damage accumulation in $KTaO_3$, *J. Materials Science* **54** [1]: 149-158 (2019).
3. R. Sachan, M. F. Chisholm, X. Ou, Y. Zhang, and W. J. Weber, Energetic ion irradiation-induced disordered nanochannels for fast ion conduction, *JOM* **71** [1]: 103-108 (2019).
4. M. L. Crespillo, J. T. Graham, F. Agulló-López, Y. Zhang, and W. J. Weber, Recent Advances on Carrier and Exciton Self-Trapping in Strontium Titanate: Understanding the Luminescence Emissions, *Crystals* **9**: 95 (2019).
5. G. Velisa, E. Wendler, L.-L. Wang, Y. Zhang, and W. J. Weber, Amorphization kinetics in strontium titanate at 16 and 300 K under argon ion irradiation, *J. Materials Science* **54** [8]: 6066-6072 (2019).
6. M. L. Crespillo, J. T. Graham, F. Agulló-López, Y. Zhang, and W. J. Weber, The Blue Emission at 2.8 eV in Strontium Titanate: Evidence for a Radiative Transition of Self-trapped Excitons from Unbound States, *Materials Research Letters* **7** [7]: 298-303 (2019).
7. X. Zhang, T. Tong, H. Xue, J. K. Keum, Y. Zhang, A. Boulle, A. Debelle, and W. J. Weber, Strain engineering 4H-SiC with ion beams, *Applied Physics Letters* **114** [22]: 221904 (2019).
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11. W. J. Weber, H. Xue, E. Zarkadoula, and Y. Zhang, Two regimes of ionization-induced recovery in $SrTiO_3$ under irradiation, *Scripta Materialia* **173**: 154-157 (2019).
12. E. Zarkadoula, Y. Zhang, and W. J. Weber, Molecular dynamics simulations of the response of pre-damaged $SrTiO_3$ and $KTaO_3$ to fast heavy ions, *AIP Advances* **10**: 015019 (2020).
13. F. X. Zhang, H. Xue, J. K. Keum, A. Boulle, Y. Zhang, and W. J. Weber, Symmetry degeneration and room temperature ferroelectricity in ion-irradiated $SrTiO_3$, *J. Physics: Condensed Matter* **32**: 355405 (2020).
14. E. Zarkadoula, G. Samolyuk, Y. Zhang, and W. J. Weber, Electronic stopping in molecular dynamics simulations of cascades in 3C-SiC, *J. Nuclear Materials* **540**: 152371 (2020).
15. L. Nuckols, M. L. Crespillo, C. Xu, E. Zarkadoula, Y. Zhang, and W. J. Weber, Coupled effects of electronic and nuclear energy deposition on damage accumulation in ion-irradiated SiC, Acta Materialia 199: 96-106 (2020).

Innovations in Immunology, Cell Biology - Structural Biology and specifically in Cell-Cell & Cell-Matrix Interactions Mediated by Integrins

by M. Amin Arnaout, Member EUAS

Short Biography

Professor of Medicine, Harvard Medical School; Director of the Leukocyte Biology and Inflammation Laboratory and the Structural Biology Program at Massachusetts General Hospital; Former Chief of the Division of Nephrology, Massachusetts General Hospital; Physician, Massachusetts General Hospital.

A. Personal Statement

I have a broad background in immunology, cell biology and structural biology, with specific expertise in cell-cell and cell-matrix interactions mediated by integrins. My major research has focused on the discovery, biology and structure of integrins and their role in inflammatory, thrombotic, fibrotic and autoimmune diseases affecting the kidney and other major organs. I also have an active research program in elucidating mechanisms of cyst formation in autosomal dominant polycystic kidney disease (ADPKD). As PI on previous and current federally-funded grants, I identified the molecular basis of leukocyte adhesion deficiency I (now known as LAD I or β2 integrin deficiency), cloned the target genes, developed knockout mice, generated monoclonal antibodies, determined the first crystal structures of integrins and used the derived structures to design a new class of anti-integrins compounds that avoid the side effects seen with current anti-integrin drugs. I established strong and durable investigative teams, bringing the proposed studies to successful conclusions, and served as senior and corresponding author on these studies. In addition, I successfully administered these projects (e.g. staffing, budget, progress reports, research protections), produced papers published in peer-reviewed high impact journals such as Science, Cell, Nature journals, PNAS, J Clin Invest, and New Engl J Med, and have served on regular and ad hoc NIH and DOD Study Sections.

B. Positions and Honors

Positions and Employment

1974-1976	*Medical resident and Chief resident, AUB Hospital, Beirut, Lebanon*
1976	*Research Fellow, Renal Division, Johns Hopkins Hospital, Baltimore, MD*
1976-1978	*Research Fellow in Immunology, Boston Children's Hospital and Harvard Med School*
1979-1980	*Clinical Fellow in Nephrology, Boston Children's Hospital/ Brigham & Women's Hospital*
1981-1988	*Instructor, Assistant-, Associate Professor of Pediatrics, Harvard Medical School*
1981-1983	*Junior attending, inpatient adult nephrology service, Brigham & Women's Hospital*
1981-1987	*Attending physician in nephrology, Boston Children's Hospital*
1988-1997	*Associate Professor of Medicine, Harvard Medical School*
1991-	*Founder and Director, Leukocyte Biology & Inflammation Laboratory, , MGH*
1996-	*Founder and Director, Structural Biology Program, MGH*
1998-	*Professor of Medicine, Harvard Medical School*
1998-2013	*Chief, Division of Nephrology, Massachusetts General Hospital*

Honors

1973	*Lange Medical Publication award for an outstanding medical student*

1981	*Young Investigator Award, NIH*
1982-1987	*Established Investigator, American Heart Association*
1986	*Elected to the American Society for Clinical Investigation (ASCI)*
1993	*Elected to the Association of American Physicians (AAP)*
1997-1998	*Program Chairman, 1998 Annual Meeting of the American Society of Nephrology*
1998-2001	*Chairman, Basic Science Committee, American Society of Nephrology*
2001	*President's Medal of Excellence- American Society of Nephrology*
2001-2002	*Member, Scientific Advisory Board, Keystone Symposia*
2001-2009	*Council Member, International Society of Nephrology*
2003	*Thabit Ben Qurrah International Award*
2004	*Richard Aster Lecture, Blood Research Institute, Milwaukee, WI*
2005	*Donald Seldon Lecture, International Society of Nephrology, Singapore*
2007-	*Principal Faculty, Harvard Stem Cell Institute, Cambridge, Massachusetts*
2007	*Donald Seldon Lecture, International Society of Nephrology, Rio de Janeiro*
2009-2013	*Elected member, Research Council, Partners HealthCare*
2010-	*Elected Member, MGH Senior Committee for Academic Promotions*
2011-2015	*Member, International Advisory Council, American University of Beirut Medical School*
2014	*Recipient of the Harvard Alumni Association Award*
2017	*Recipient of the International Kuwait Prize in Applied Medical Sciences*
2018	*Recipient of Homer W Smith Award from the American Society of Nephrology*
2019	*Elected to the American Clinical and Climatological Association.*

In 1867, Julius F. Cohnheim described in masterful details the process of leukocyte migration across vascular endothelium within the tongue of a live frog in response to an inflammatory signal, using a very simple light microscope. He noticed that leukocytes first come to a halt, line up the wall of venules, and then creep across the vascular wall into the extravascular space. Years later, Metchnikoff proposed that the physiologic function of these extravasated cells is to "eat" invading pathogens. His "phagocytosis" theory was in conflict with Paul Ehrlich's "humoral" theory that stated that serum-derived "magic bullets" (now called antibodies and complement) are all what is needed to kill pathogens. Both shared the Nobel Prize in 1908 for describing the humoral and cellular arms of inflammation. However, the molecular basis of leukocyte phagocytosis and extravasation remained unknown.

In 1979, we became interested in elucidating the basis for recurrent life-threatening bacterial infections in a pediatric patient. In a series of studies over the next two years, we traced the molecular basis of this disease to impaired phagocyte adhesion, manifested by defective phagocytosis and extravasation. We found that the patient's phagocytes were missing a previously unknown plasma membrane glycoprotein (gp) complex of ~150 kDa (gp150), and that the disease is inherited on an autosomal recessive basis (Lead Article in the *New England Journal of Medicine*, 1982). The disease became later known as Leukocyte Adhesion Deficiency type I (LAD I). Further work showed that this gp150 complex comprises α-subunits of four cell surface glycoproteins that share a common 94 kDa β-subunit, collectively known now as β2 integrins (*J Clin Invest*, 1983, 1984a, 1984b, 1984c, 1984d, *Eur J Immunol*, 1985, *J Clin Invest*, 1987). These glycoproteins participate in selective (e.g. phagocytosis, *J Clin Invest*, 1983) as well as overlapping leukocyte functions (e.g. transendothelial or transepithelial migration, *J. Cell Phys*, 1989, *J. Clin Invest*, 1991). We traced the inherited defect in LAD I to mutations in the common β subunit (*J Clin Invest 1987, 1990*, *J Biol Chem, 1992*) that prevent its noncovalent

association with each of the individual α subunits, a process required for normal surface expression of these heterodimers We also demonstrated the potential therapeutic value of blocking β2 integrins in acute inflammatory states (*New England Journal of Medicine 1985*; *Immunol Rev, 1990; Am J Phys, 1991; J Cell Biol 1992; J Cell Biol, 1993*). In parallel studies, we isolated (*BBA*, 1986) and cloned (*Proc. Natl Acad Sciences*, 1988; *J Cell Biol*, 1988) the α subunit of the major phagocytic integrin expressed on human neutrophils, CD11b, showed that it is a type I membrane glycoprotein and that it contains a von Willebrand Factor (vWF) A type domain (hence the name αA domain) in its extracellular segment, then showed that the αA domain that is responsible for divalent-cation dependent ligand binding in β2 integrins (*Cell*, 1993).

With the realization that overactive integrins contribute to many common diseases including thrombotic, inflammatory, autoimmune, and fibrotic disorders, the pharmaceutical industry raced to make and successfully introduce RGD-based small molecules and cyclic peptides as well as mAb drugs, which focused on mitigating coronary thrombosis and certain autoimmune diseases (multiple sclerosis and inflammatory bowel disease). We, however, focused on better understanding of the structural basis of integrin activation and pioneered a structure-based approach to integrin biology that culminated in our determination of the first crystal structures of the integrin αA domain in its active (ligand bound) and inactive conformations (*Cell*, 1995; *Structure*, 1995). We then showed that it is feasible to express and purify a functional integrin ectodomain (*Proc. Natl Acad Sciences*, 1991), which made it feasible for us to determine the first crystal structure of the large integrin ectodomain in its inactive state and also in complex with a ligand-mimetic cyclic heptapeptide (*Science*, 2001; *Science* 2002; *J Cell Biol*, 2009). These crystal structures revealed an unexpected bent conformation of the integrin that now forms a basis for current understanding of integrin activation and proadhesive signaling (reviewed in *F1000Res*, 2016). These scientific achievements were hailed on the pages of *Science* and *Nature* journals as "one of those spectacular results that will change a field", as "concomitantly advancing the field one enormous stride, and as a "MIDAS touch to cell signaling" (*Nature Struc Biol, '98; Science vol 293, 2001; Science vol 294, 2001; Nature Reviews, 2002*). These achievements were also covered in the lay press (*New York Times, 1993; Harvard Gazette, 2014, MGH News 2016, MGH News 2017*).

With the widespread use of anti-integrin therapeutics, it became clear that these drugs can cause serious side effects since they act as partial agonists, i.e. they elicit the same activating conformational changes in the integrin as physiologic ligands. Such changes in platelet integrin αIIbβ3, for example, inhibit clot retraction and elicit prolonged expression of integrin neoepitopes that are recognized by natural antibodies in some patients, both accounting for the severe bleeding seen in patients receiving parenteral anti-αIIbβ3 drugs. When these compounds were administered orally for chronic use, activation of αIIbβ3 persists after these compounds have dissociated, allowing it to now bind circulating fibrinogen, causing paradoxical thrombosis and increased mortality in patients, which lead to failed clinical trials. These finding lead to the conclusion that partial agonism and antagonism of integrins are inseparable, resulting in development of anti-thrombosis drugs targeting other receptors upstream of integrins, but these continue to cause bleeding in treated patients.

In a series of studies, we found that it is possible to effectively antagonize an integrin without paradoxically activating it. We initially raised a ligand mimetic (orthosteric) mAb against CD11b, the archetypal innate immune receptor (*J. Immunol*., 2002), and found that this mAb stabilized CD11b in the inactive conformation (*J. Immunol, 2011*) and prevented the conformational switch of the integrin to the activated state in human neutrophils.

Crystal structure determination of this mAb/CD11b complex elucidated the atomic basis of this unexpected effect (*J. Immunol, 2011*). This mAb prevented fibroinflammatory kidney failure in cynomolgus monkeys (*Nature Comm,* 2017), establishing it as a first-in-class "pure" orthosteric integrin inhibitor. More recently, we have developed pure antagonists to other integrins. Our crystal structure of αvβ3 in complex with a modified high-affinity version of its fibronectin ligand, the 10th type III RGD-containing domain (hFN10) revealed that hFN10-bound αvβ3 also remained in its inactive conformation (*Nature Struc Mol Biol, 2014*). This structure was then used to generate a small molecule pure antagonist of αvβ3 (*ACS Pharmacol Transl Sci, 2019*) and of αIIbβ3 by converting the partial agonist drug Tirofiban (Aggrastat®) into a pure antagonist (*Nature Comm, 2020*). In head-to-head comparisons, the pure antagonist was as effective as Tirofiban in blocking thrombosis *in vivo* but in sharp contrast, it did not cause excessive bleeding seen with Tirofiban (*Nature Comm, 2020*). Collectively, these studies now provide a structural basis for designing small molecule pure orthosteric antagonists of other integrins.

Previous efforts in my laboratory have also led to the first identification of C3 nephritic factor as an autoantibody to the alternative pathway C3 convertase (*J Immunol, 1977*; *New England Journal of Medicine, 1977)*. This work changed the prevailing concept of how complement activation is initiated, and lead to an assay for measuring C3Nef, which is used in the differential diagnosis of immune-mediated kidney disease. We also characterized complement receptor type 1 (*J Immunol, 1981)* and elucidated its novel role as repressor of complement activation (*Eur J Immunol, '83*), studies that contributed to better understanding of the role of complement in renal disease and its therapeutic targeting. We also identified the Wegener's Granulomatosis autoantigen, responsible for one form of systemic vasculitis, as a novel serine proteinase (*Blood, 1990*), which lead to development of diagnostic ELISA test for this disease. We also discovered that polycystin 1, the membrane protein defective in Autosomal Dominant Polycystic Kidney Disease (ADPKD) plays an essential role in vascular integrity (*Proc. Natl Acad Sciences, 2000*), and demonstrated that polycystin 2, a second protein defective in ADPKD, is a TRP-like ion channel (*Proc. Natl Acad Sciences, 2001*). My work has been continuously funded by NIH since 1982 and has been recognized by my election to prestigious academic societies, and through several awards including the 2017 Kuwait Prize in Applied Medical Sciences and the 2018 Homer W. Smith Award presented by the American Society of Nephrology to "an individual who made outstanding contributions which fundamentally affect the science of nephrology."

While conducting several of the above studies, I also served as Chief of the Division of Nephrology at the Massachusetts General Hospital for 15 years (1998-2013), building its clinical inpatient and outpatient services and its basic and clinical research programs. I expanded Division staff to more than 100 clinicians, scientists, educators, and advanced the Division to become a premier academic center for patient care, training and research in nephrology, reflected in its highest rankings by *US New and World Reports.* As Chief and Program Director of T32 NIH training grant, I trained and supervised more than 130 clinical and research fellows, MDs and/or PhDs, many assuming leading positions in academic institutions and in biotech industry.

Top 10 References

1. Arnaout MA, Pitt J, Cohen HJ, Melamed J, Rosen FS, Colten HR. Deficiency of a granulocyte-membrane glycoprotein (gp150) in a boy with recurrent bacterial infections. ***N Engl J Med.*** 306(12):693-9, 1982.

2. Arnaout MA, Spits H, Terhorst C, Pitt J, Todd RF. Deficiency of a leukocyte surface glycoprotein (LFA-1) in two patients with Mol deficiency. Effects of cell activation on Mol/LFA-1 surface expression in normal and deficient leukocytes. ***J. Clin. Invest***. 74, 1291-1300, 1984.
3. Michishita M, Videm V, Arnaout MA. A novel divalent cation-binding site in the A domain of the beta 2 integrin CR3 (CD11b/CD18) is essential for ligand binding. ***Cell***. 72(6):857-67, 1993.
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5. Xiong JP, Stehle T, Diefenbach B, Zhang R, Dunker R, Scott DL, Joachimiak A, Goodman SL, Arnaout MA. Crystal structure of the extracellular segment of integrin αvβ3. ***Science***. 294(5541):339-45, 2001.
6. Xiong JP, Stehle T, Zhang R, Joachimiak A, Frech M, Goodman SL, Arnaout MA. Crystal structure of the extracellular segment of integrin αvβ3 in complex with an Arg-Gly-Asp ligand. ***Science***. 296(5565):151-5, 2002.
7. Mahalingam B, Ajroud K, Alonso JL, Anand S, Adair BD, Horenstein AL, Malavasi F, Xiong JP, Arnaout MA. Stable coordination of the inhibitory Ca^{2+} ion at the metal ion-dependent adhesion site in integrin CD11b/CD18 by an antibody-derived ligand aspartate: implications for integrin regulation and structure-based drug design. ***J Immunol***. 187(12):6393-401, 2011.
8. Van Agthoven JF, Xiong JP, Alonso JL, Rui X, Adair BD, Goodman SL, Arnaout MA. Structural basis for pure antagonism of integrin αvβ3 by a high-affinity form of fibronectin. ***Nat Struct Mol Biol*** 21(4):383-8, 2014.
9. Dehnadi A, Benedict Cosimi A, Neal Smith R, Li X, Alonso JL, Means TK, Arnaout MA. Prophylactic orthosteric inhibition of leukocyte integrin CD11b/CD18 prevents long-term fibrotic kidney failure in cynomolgus monkeys. ***Nat Commun.*** 8:13899, 2017.
10. Adair BD, Alonso JL, van Agthoven J, Hayes V, Sook Ahn H, Yu I-S, Lin S-W, Xiong JP, Poncz M, Arnaout MA. Structure-guided design of novel orthosteric inhibitors of integrin αIIbβ3 that prevent thrombosis but preserve hemostasis. ***Nat Commun.*** 11:398, 2020.

Developments in Mathematical Analysis & Partial Differential Equations

by Vladimir Maz'ya, Member EUAS

Short Biography

Dept. of Mathematical Sciences, University of Liverpool, Liverpool L69 7ZL, UK, Honorary Senior Fellow

Dept. of Mathematics, Linköping University, SE-581 83 Linköping, Sweden, Professor Emeritus

Main research interests

Linear and nonlinear PDEs - Asymptotic and numerical methods for PDEs, including homogenization and boundary elements - Spectral theory - Harmonic analysis - Approximation theory - Wavelets - Elasticity theory - Function spaces - Ill-posed problems - Nonlinear potential theory - Fluid mechanics - History of mathematics

Education

1965 Sci. D. in Mathematics Leningrad State University, Russia
1962 Ph. D. in Mathematics Moscow State University, Russia
1960 MS in Mathematics Leningrad State University, Russia

Employment

2010 { Honorary Senior Fellow, Department of Mathematical Sciences, University of Liverpool
September 2003 - 2010 { Professor, Department of Mathematical Sciences, University of Liverpool
January, 2004 - June 2008 Professor, Department of Mathematics, Ohio State University
September - November 2003 Senior Fellow, Schrödinger Institute, Vienna
January - June 2003 Visiting Stone Professor, Northeastern University, Boston
March - May 2002 Visiting position Maitre des Recherches, Institute Henri Poincare, Paris
September - December 1994 Visiting position of Maitre des Recherches, Ecole Polytechnique, Palesaux
2003 { Professor Emeritus, Department of Mathematics, Linköping University, Sweden
1993 - 2002 Professor, Department of Mathematics, Linköping University, Sweden
1990 - 1993 Associate Professor, Department of Mathematics, Linköping University, Sweden
1986-1990 Head of Laboratory of Mathematical Models in Mechanics, Leningrad Institute of Engineering
Studies of Academy of Sciences USSR
1968-1972 Professor, Department of Mathematics, Leningrad Shipbuilding Institute
1964-1986 Senior Research Scientist, Mathematics and Mechanics Institute, Leningrad State University
1960-1964 Junior Research Scientist, Mathematics and Mechanics Institute, Leningrad University

Honours and Awards

October 2013, Foreign Member of the Georgian National Academy of Sciences
2012 elected fellow of the American Mathematical Society.
July 2009, Senior Whitehead Prize of the London Mathematical Society.
May 2004, The Celsius Gold Medal of the Royal Society of Sciences at Uppsala.

March 2003, Verdaguer Prize of the French Academy of Sciences.
April 2002, Member of the Royal Swedish Academy of Sciences.
5th March, 2001, Corresponding Fellow of the Royal Society of Edinburgh.
November 1999, Humboldt Research Prize.
1990 Doctor honoris causa of the University of Rostock, Germany.
1962 Prize of the Leningrad Mathematical Society, Russia.

Publications in honour of Vladimir Maz'ya

-Around the Research of Vladimir Maz'ya I - III: Function Spaces, Partial Differential Equations, Analysis Applications, International Mathematical Series, Vol. 11-13 A. Laptev (Ed.), Springer, 2010.
-Analysis, Partial Differential Equations and Applications, The Vladimir Maz'ya Anniversary Volume, Series: Operator Theory: Advances and Applications, Vol. 193, A. Cialdea, F. Lanzara, P.E. Ricci (Eds.), Birkhäuser 2009.
-Perspectives in Partial Differential Equations, Harmonic Analysis and Applications: A Volume in Honor of Vladimir G. Maz'ya's 70th Birthday, Proceedings of Symposia in Pure Mathematics, AMS, 2008.
-M.V. Anolik et al, Vladimir Gilelevich Maz'ya (On the Occasion of His 70th Anniversary), Vestnik Sankt-Peterburgskogo Universiteta. Seriya 1. Matematika, Mekhanika, Astronomiya, no. 4 (2008), 3-6.
-M. S. Agranovich et al, Vladimir Gilelevich Maz'ya (on his 70th birthday), Russian Math. Surveys 63:1 (2008), 189 -196.
-M.S.Agranovich et al, Vladimir G. Maz'ya. On the occasion of his 65th anniversary, Russian J. of Math. Physics, 10:3 (2003), 239-244.
-The Maz'ya Anniversary Collection, Rossmann, J., Takac, P., Wildenhain, G. (Eds.), Birkhäuser Verlag, 1999:Volume 1: On Maz'ya's Work in Functional Analysis, Partial Differential Equations and Applications. Volume 2: Rostock Conference on Functional Analysis, Partial Differential Equations and Applications.
-Mathematical Aspects of Boundary Element Methods, dedicated to Vladimir Maz'ya on the occasion of his 60th birthday, M. Bonnet, A.-M. Sändig and W. Wendland (Eds.), Chapman and Hall/CRC Research Notes in Mathematics, London, 1999.
-Eidus, D. et al, Mathematical work of Vladimir Maz'ya (on the occasion of his 60th birthday), Funct. Differ. Equ. 4 (1997), no. 1-2 (1998), 3-11.

Research Interests

Vladimir G. Maz'ya, born 31 December 1937, is a Russian-born Swedish mathematician, hailed as "one of the most distinguished analysts of our time" and as "an outstanding mathematician of worldwide reputation", who strongly influenced the development of mathematical analysis and the theory of partial differential equations.

Mazya's early achievements include: his work on Sobolev spaces, in particular the discovery of the equivalence between Sobolev and isoperimetric/isocapacitary inequalities (1960), his counterexamples related to Hilbert's 19th and Hilbert's 20th problem (1968), his solution, together with Yuri Burago, of a problem in harmonic potential theory (1967) posed by Riesz & Szőkefalvi-Nagy (1955, chapter V, § 91), his extension of the Wiener regularity test to p–Laplacian and the proof of its sufficiency for the boundary regularity. Maz'ya solved Vladimir Arnol'd's problem for the oblique derivative boundary value problem (1970) and Fritz John's problem on the oscillations of a fluid in the presence of an immersed body (1977).

In recent years, he proved a Wiener's type criterion for higher order elliptic equations, together with Mikhail Shubin solved a problem in the spectral theory of the Schrödinger operator formulated by Israel Gelfand in 1953, found necessary and sufficient conditions for the validity of maximum principles for elliptic and parabolic systems of PDEs and introduced the so–called approximate

approximations. He also contributed to the development of the theory of capacities, nonlinear potential theory, the asymptotic and qualitative theory of arbitrary order elliptic equations, the theory of ill-posed problems, the theory of boundary value problems in domains with piecewise smooth boundary.

Because of Maz'ya's ability to give complete solutions to problems which are generally considered as unsolvable, Fichera once compared Maz'ya with Santa Rita, the 14th century Italian nun who is the Patron Saint of Impossible Causes.— *Alberto Cialdea, Flavia Lanzara and Paolo Emilio Ricci, (Cialdea, Lanzara & Ricci 2009, p. xii).*

Maz'ya authored/coauthored more than 550 publications, including 20 research monographs. Several survey articles describing his work can be found in the book (Rossmann, Takáč & Wildenhain 1999a), and also the paper by Dorina and Marius Mitrea (2008) describes extensively his research achievements, so these references are the main ones in this section: in particular, the classification of the research work of Vladimir Maz'ya is the one proposed by the authors of these two references.

Maz'ya is the author of tales for children and grown-ups published in Moscow in Russian (https://users.mai.liu.se/vlama82/books-skazki/index.html). His reminiscences were published in English by Birkhauser (https://www.springer.com/gp/book/9783319018089) and in Russian by Aleteya (https://www.facebook.com/430141753719884/posts/3243995269001171/).

Honors

In 1962 Maz'ya was awarded the "Young Mathematician" prize by the Leningrad Mathematical Society, for his results on Sobolev spaces: he was the first winner of the prize.—In 1990 he was awarded an honorary doctorate from Rostock University. In 1999, Maz'ya received the Humboldt Prize. He was elected member of the Royal Society of Edinburgh in 2000, and of the Swedish Academy of Science in 2002.— In March 2003, he, jointly with Tatyana Shaposhnikova, was awarded the Verdaguer Prize by the French Academy of Sciences.–On 31 August 2004 he was awarded the Celsius Gold Medal, the Royal Society of Sciences in Uppsala's top award, "*for his outstanding research on partial differential equations and hydrodynamics*".–He was awarded the Senior Whitehead Prize by the London Mathematical Society on 20 November 2009.–In 2012 he was elected fellow of the American Mathematical Society.On 30 October 2013 he was elected foreign member of the Georgian National Academy of Sciences.

Starting from 1993, several conferences have been held to honor him: the first one, held in that year at the University of Kyoto, was a conference on Sobolev spaces.–On the occasion of his 60th birthday in 1998, two international conferences were held in his honor: the one at the University of Rostock was on Sobolev spaces, while the other, at the École Polytechnique in Paris,–was on the boundary element method. He was invited speaker at the International Mathematical Congress held

in Beijing in 2002: his talk is an exposition on his work on Wiener–type criteria for higher order elliptic equations. Other two conferences were held on the occasion of his 70th birthday: "*Analysis, PDEs and Applications on the occasion of the 70th birthday of Vladimir Maz'ya*" was held in Rome, while the "*Nordic – Russian Symposium in honour of Vladimir Maz'ya on the occasion of his 70th birthday*" was held in Stockholm. On the same occasion, also a volume of the Proceedings of Symposia in Pure Mathematics was dedicated to him. On the occasion of his 80th birthday, a "Workshop on Sobolev Spaces and Partial Differential Equations" was held on 17–18 May 2018 was held at the Accademia Nazionale dei Lincei to honor him. On the 26–31 May 2019, the international conference "Harmonic Analysis and PDE" was held in his honor at the Holon Institute of Technology.

Impovements in Analysis, Probability, Wavelets, Signals & Fractals

by Palle Jorgensen, Member EUAS

Short Biography

Professor of mathematics, teaches at the University of Iowa, Iowa City, USA; and has taught at Stanford University, and at the University of Pennsylvania.,-- funding from the Natl. Sci. Foundation,-- his research papers are in international scientific journals,-- math, both pure and applied (operator algebras, and harmonic analysis), and mathematical physics (quantum theory). Recent research: wavelet theory, subdivision algorithms, spectral-tile duality, scaling and fractals. For a 2002 wavelet book, see
http://www.math.uiowa.edu/~jorgen
Specialties: *Analysis and Probability: Wavelets, Signals, Fractals (Graduate Texts in Mathematics) (September 19, 2006)*
Wavelets through a Looking Glass (Applied and Numerical Harmonic Analysis) (July 12, 2002)
Professor Palle Jorgensen: (1) Teaching, mentoring; (2) scholarship, research publications and books; and (3) service, to the University and to the profession.
Education*. Highest Degree, PhD Mathematics, 1973, Aarhus University, Denmark. Recognition. Jorgensen is an elected member of the Danish Academy of Natural Sciences, the Society of the EU Academy of Sciences, and the New York Academy of Sciences.*
1984-Present: Professor, Department of Mathematics, University of Iowa.
Professional and Academic Positions before Univ of Iowa, reverse chronology:
1982-84: Visiting Associate Professor, Department of Mathematics, University of Pennsylvania.
1980-82: Associate Professor, Mathematics Institute, Aarhus University, Denmark, on leave from Stanford the first year.
1977-80: Assistant Professor, Department of Mathematics, Stanford University. (The PhD students from Jorgensen's Stanford graduate courses included Peter Sarnak (now IAS, Princeton), and Ruth Williams (UCSD), now both members of the US Academy of Sciences.)
1973-77: Postdoctoral Research Fellow, University of Pennsylvania, support from the Danish Natural Science Research Council; (on NSF MCS 77-02831, R.V. Kadison, PI).

Scholarship, Research Publications and Books

Both before and after joining the University of Iowa faculty, Jorgensen held continuous **NSF** support, as co-PI or as PI; this continued up to 2017. This includes **NSF funded collaborative research teams**: Jorgensen was co-PI on two FRG grants, and three bi-national grants. Details: *Focused Research Group* (FRG) grants. (FRG is an NSF program, collaborative teams of PIs, made up from multiple Universities.) Jorgensen has also been co-PI on three separate bi-national funded teams, Norway, Europe, and Israel. (So, NSF together with the respective foreign funding sources.)

CBMS in 2018. Jorgensen gave the ten invited CBMS/NSF lectures in harmonic analysis.**:** Jorgensen was the Principal Lecturer in a **CBMS meeting titled**

"*Harmonic analysis: smooth and non-smooth*". Jorgensen gave the 10 lectures at ISU, and he wrote them up in as an AMS book, *vol 128 in the CBMS series*. **Title**: *Harmonic Analysis: Smooth and Non-Smooth*; published in the **CBMS (Regional Conference Series in Mathematics) book series**, Volume: 128; 2018; AMS & NSF.

Total of 340 publications and books. Scholarship/publications by numbers, listed in *MathSciNet* (as of 10/28/2020).
Total Publications count: 340.

Total Related Publications: 16.

Citation count (MSN): 3,025. *Google Scholar* (citations and indices): total citations 20,305; h-index 43; i-index 193.

List of Twelve books by Jorgensen (2 more accepted, one by Springer, and another by the AMS):

Operator commutation relations, Commutation relations for operators, semigroups, and resolvents with applications to mathematical physics and representations of Lie groups (1984), Dordrecht; by Palle E T Jorgensen and Robert T Moore.

Operators and representation theory. Canonical models for algebras of operators arising in quantum mechanics (1988), Elsevier, by Palle E T Jorgensen. (Now in 3rd edition in Dover.)

Iterated Function Systems and Permutation Representations of the Cuntz Algebra (1999), AMS, Memoirs; by Ola Bratteli and Palle E T Jorgensen.

Wavelets through a looking glass. The world of the spectrum (2002), Springer; by Ola Bratteli and Palle E T Jorgensen.

Representation Theory and Numerical AF-Invariants: The Representations and Centralizers of Certain States on Od (2004), AMS Memoirs; by Ola Bratteli, Palle E T Jorgensen and Vasyl Ostrovskyi.

Analysis and probability: wavelets, signals, fractals (2006), Springer, GTM v 234; by Palle E T Jorgensen.

Iterated Function Systems, Moments, and Transformations of Infinite Matrices (2011), AMS Memoirs; by Palle E T Jorgensen, Keri A Kornelson and Karen L Shuman.

Extensions of positive definite functions. Applications and their harmonic analysis (2016), Springer LNM; by Palle E T Jorgensen, Steen Pedersen, and Feng Tian.

Non-commutative analysis (2017), World Scientific; by Palle E T Jorgensen and Feng Tian.

Transfer operators, endomorphisms, and measurable partitions (2018), Springer, LNM; by Sergey Bezuglyi and Palle E T Jorgensen.

Harmonic analysis. Smooth and non-smooth (2018), AMS CBMS; by Palle E T

Jorgensen.

Infinite-dimensional analysis: Operators in Hilbert space, stochastic calculus via representations and duality theory; World Scientific https://doi.org/10.1142/11980 Feb 27, 2021; by Palle Jorgensen and James Tian.

Publications in research topic-journals, all highly ranked; for the full list see *MathSciNet***.** Jorgensen's 340 publications have appeared in refereed and competitive journals.

Synergistic

Jorgensen had 29 PhD students, and he is an editor of several top journals in applied mathematics. Has mentored many undergraduate research students, as well as 9 postdocs. *Memberships*: Amer Math Soc, the New York Academy of Science, the Danish Academy of Science. Jorgensen's research focuses on such areas of mathematics that have found use in physics and in engineering: In *math physics*, coherent states, scattering theory, quantum fields, symmetry, reflection positivity. In *engineering*, signal and image processing, representation of signals, time-frequency analysis, wavelet representations and algorithms, and bit-quantization. His research papers appeared in state-of-the-art applied mathematics journals. *Keywords & Amer Math Soc classification codes*: Stochastic analysis (37), approximations and expansions, wavelets (41), harmonic analysis (43), machine learning (60), QM (81). *Sample funding history*: NSF funding. Jorgensen, co-PI is, Bi-National grant, US-Israel, which ran out in the spring of 2010-17. Held collaborative NSF grants, one collaborative USA, and separately, a US-Israel grant. In the fall of 2009, he won a three-year Collaborative Research Proposal with Prof Dorin Dutkay as co-PI. Jorgensen co-directed the research of several of our VIGRE graduate students. *Citation numbers*. As of September 2020, the Amer Math Soc *MathSciNet* list for Jorgensen has 343 publications, research papers in refereed journals; there are more as *MathSciNet* does not list all math phys papers.

Extensive interdisciplinary collaborations, multiple departments in CLAS, multiple University of Iowa colleges (business, engineering, and bio-statistics), and major Universities around the World. Focused on a host of applications: stochastic analysis, and addressing industry, with view to financial services industries, risk management, energy sustainability issues, homogenization of multiscale-random media, medical imaging, data mining, and energy efficiency/smart grids. Stochastic analysis and related disciplines play a significant role in almost every branch of science and engineering.

Improvements in Biomedical Materials & Clinical Biochemistry

by Pankaj Vadgama, Member EUAS

Short Biography

CURRENT APPOINTMENTS

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

ACADEMIC QUALIFICATIONS

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

ACADEMIC APPOINTMENTS

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

Editorial Board Positions

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

National/International Committees

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

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

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

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

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

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

Research Interests

His main research interest has been in the development of electrochemical devices for

near patient diagnostic systems, in particular, bio- and chemical sensors for the *in vivo* and *ex vivo* monitoring of ions, oxygen and metabolites, respectively. The underpinning research work has been sensor materials design and in particular the design of polymeric membranes for the control of mass transport and device interfacial biocompatibility. Other research has focussed on sweat and saliva monitoring, during exercise, computation models for solute mass transport measurement at polymeric membrane barriers, silver nanocomposites for microbially resistant surfaces, textile ion sensors for on body monitoring, and enhanced strength bone adhesive, spider silk as tissue scaffolds and microfluidics: *in vitro* for membrane formation and *in vivo* for enhanced biosensor tissue biocompatibility and non-invasive monitoring of tissue biochemistry.

N. Baishya, K. Budidha, M. Mamouei, M. Qassem, P. Vadgama and P. A. Kyriacou, "Near Infrared Spectrometric Investigations on the behaviour of Lactate," ***2019 41st Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC),*** **Berlin, Germany, 2019, pp. 5769-5772, doi: 10.1109/EMBC.2019.8857833.**

Abstract

In patients with life-threatening illnesses, the metabolic production and disposal of lactate are impaired, which leads to a build-up of blood lactate. In critical care units, the changes in lactate levels are measured through intermittent, invasive, blood sampling and in vitro assay. Continuous monitoring is lacking, yet such monitoring could allow early assessment of severity and prognosis to guide therapy. Currently, there is no routine means to measure lactate levels continuously, particularly non-invasively. The motivation of this study was to understand the interaction of lactate with light in the Near Infra Red (NIR) region of the electromagnetic spectrum. This was to create an opportunity to explore the possibility of a non-invasive sensing technology to monitor lactate continuously.In vitro studies were performed using solution samples with varying concentration levels of sodium lactate in isotonic Phosphate Buffer Solution (PBS) at constant pH (7.4). These samples were prepared using stoichiometric solution compositions and spectra for each sample were taken using a state-of-the-art spectrometer in the NIR region. The spectra were then analysed qualitatively by 2D correlation analysis, which identified the regions of interest. Further analysis of these regions using linear regression at four randomly selected wavelengths showed bathochromic shifts, which, moreover, showed systematic variation correlating with lactate concentration.

M. Mamouei, M. Qassem, K. Budidha, N. Baishya, P. Vadgama and P. A. Kyriacou, "Comparison of a Genetic Algorithm Variable Selection and Interval Partial Least Squares for quantitative analysis of lactate in PBS," ***2019 41st Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC),*** **Berlin, Germany, 2019, pp. 3239-3242, doi: 10.1109/EMBC.2019.8856765.**

Abstract

Blood lactate is an important biomarker that has been linked to morbidity and mortality of critically ill patients, acute ischemic stroke, septic shock, lung injuries, insulin resistance in diabetic patients, and cancer. Currently, the clinical measurement of blood lactate is done by collecting intermittent blood samples. Therefore, noninvasive, optical measurement of this significant biomarker would lead to a big leap in healthcare. This study, presents a quantitative analysis of the optical properties of lactate. The benefits of wavelength selection for the development of accurate, robust, and interpretable predictive models have been highlighted in the literature. Additionally, there is an obvious, time- and cost-saving benefit to focusing on narrower segments of the electromagnetic spectrum in practical applications. To this end, a dataset consisting of 47 spectra of Na-lactate and Phosphate Buffer Solution (PBS) was produced using a Fourier transform infrared spectrometer,

and subsequently, a comparative study of the application of a genetic algorithm-based wavelength selection and two interval selection methods was carried out. The high accuracy of predictions using the developed models underlines the potential for optical measurement of lactate. Moreover, an interesting finding is the emergence of local features in the proposed genetic algorithm, while, unlike the investigated interval selection methods, no explicit constraints on the locality of features was imposed. Finally, the proposed genetic algorithm suggests the formation of α-hydroxy-esters methyl lactate in the solutions while the other investigated methods fail to indicate this.

N. Baishya, M Momouei, K Budidha, M Qassem, P Vadgama and P A Kyriacou Journal of Near Infrared Spectroscopy 2020, Vol. 28(5–6) 328–333

Abstract

Lactic acidosis is commonly observed in various disease states in critical care and can be adopted as a hemodynamic biomarker, as well as a target for therapy. pH is the main biomarker for the diagnosis of acid–base disorders and is currently measured utilizing invasive blood sampling techniques. Therefore, there is a need for a non-invasive and continuous technology for the measurement of pH and lactate levels. In this work, near infrared spectroscopy is explored as a technique for investigating lactic acidosis. In-vitro studies on 20 isotonic phosphate buffer solutions of varying pH with constant lactate concentration (2 mmol/L) were performed. The whole near infrared spectrum (800–2600 nm) was then divided into four parts for analysis: (a) water absorption peaks, (b) 1000–1250 nm, (c) 1700–1760 nm, and (d) 2200–2400 nm. The water absorption peaks showed a linear variation with the changes in pH in the spectra. The range from 1700–1760 nm showed good correlation with calculated values for lactate ionization, with the changes in pH. However, the region from 2200–2400 nm showed a reverse correlation with respect to the concentration changes of lactate and a distinction could be made from pH 6–7 and 7–8. This study successfully identifies wavelengths (1233 nm, 1710 nm, 1750 nm, 2205 nm, 2319 nm, and 2341 nm) which can be directly correlated to lactic acidosis. Knowledge from this study will contribute toward the development of lactate-based pH monitoring optical sensor for critical care.

Vadgama, P. Monitoring with In Vivo Electrochemical Sensors: Navigating the Complexities of Blood and Tissue Reactivity. Sensors 2020, 20, 3149

Abstract

The disruptive action of an acute or critical illness is frequently manifest through rapid biochemical changes that may require continuous monitoring. Within these changes, resides trend information of predictive value, including responsiveness to therapy. In contrast to physical variables, biochemical parameters monitored on a continuous basis are a largely untapped resource because of the lack of clinically usable monitoring systems. This is despite the huge testing repertoire opening up in recent years in relation to discrete biochemical measurements. Electrochemical sensors offer one of the few routes to obtaining continuous readout and, moreover, as implantable devices information referable to specific tissue locations. This review focuses on new biological insights that have been secured through in vivo electrochemical sensors. In addition, the challenges of operating in a reactive, biological, sample matrix are highlighted. Specific attention is given to the choreographed host rejection response, as evidenced in blood and tissue, and how this limits both sensor life time and reliability of operation. Examples will be based around ion, O_2, glucose, and lactate sensors, because of the fundamental importance of this group to acute health care.

N. Baishya, M Momouei, K Budidha, M Qassem, P Vadgama and P A Kyriacou Molecules 2020, 25, 3695

Abstract

Quantification of lactate/lactic acid in critical care environments is essential as lactate serves as an important biochemical marker for the adequacy of the haemodynamic circulation in shock and of cell respiration at the onset of sepsis/septic shock. Hence, in this study, ATR-FTIR was explored as a potential tool for lactate measurement, as the current techniques depend on sample preparation and fails to provide rapid response. Moreover, the effects of pH on PBS samples (7.4, 7, 6.5 and 6) and change in solution conditions (PBS to whole blood) on spectral features were also investigated. A total 189 spectra from five sets of lactate containing media were obtained. Results suggests that lactate could be measured with more than 90% accuracy in the wavenumber range of 1500–600 cm−1 . The findings of this study further suggest that there exist no effects of change in pH or media, when estimating lactate concentration changes in this range of the Mid-IR spectral region.

M Feroz and P Vadgama Electroanalysis 2020, 32, 2361 – 2386 Molecular Imprinted Polymer Modified Electrochemical Sensors for Small Drug Analysis: Progress to Practical Application

Abstract

Molecular imprinted polymers (MIPs) are tailor made from synthetic polymers and designed to mimic the recognition properties of natural biological affinity molecules. MIPs incorporate binding motifs complementary to target organic molecule shape and functional groups in order to mimic the complex binding surfaces of natural macromolecules. This confers selectivity and specificity, with the added advantage of artificial MIP polymer stability and ready adaptability to the fabrication and creation of miniaturised affinity interfaces for electrochemical sensing and extra-laboratory testing. Their generic capability as robust sorbent phases for drug extraction and concentration allows for targeted, interfacial interrogation by the active electrochemical surface. A wide range of electrochemical sensing strategies has also been advanced in recent years, which is covered by this review. The review covers MIP functional principles, examples of MIP preparative routes and final assay outcomes for the measurement of small molecule drugs of biomedical, and also of potential environmental relevance. Some small molecules as examples of toxin and contaminant measurement are also given. A historic background to MIP development is provided, but the review mainly focuses on electrochemical sensor advances in the last five years.

S Anastasova, A-M Spehar-Délèze, R M Kwasnicki, G-Z Yang and P Vadgama Electrochemical Monitoring of Subcutaneous Tissue pO2 Fluctuations during Exercise Using a Semi-implantable Needle Electrode Electroanalysis 2020, 32, 2393 – 2403

Abstract

Semi-implantable needle oxygen electrodes were used for forearm subcutaneous monitoring in human subjects undertaking high intensity cycling and fist clenching exercise. pO(2) variations in the range between 40 and100 mm Hg oxygen were seen. Superimposed on these were paradoxical rises in subcutaneous pO(2), of up to 100 mm Hg which paralleled the scale of the exercise. This was indicative of increased blood flow through skin. Triton X-100 incorporated into the sensor polyurethane membranes helped to give faster responses and reduced the possibility of biofouling and drift. The sterilizable system, free from internal electrolyte film appears promising for future clinical monitoring.

Functionalized Cellulose Nanocrystals for Advanced Drilling Fluids with Thermo-thickening & Salt-tolerant Performance

by Qinglin Wu, Member EUAS

Short Biography

A. EDUCATION

1993	*Ph.D. in Wood Science & Engineering, Oregon State Univ, Corvallis, Oregon.*
1989	*Master Eng. Sci. in Mechanical Engineering, University of Tasmania, Australia.*
1983	*BS in Agricultural Engineering, Henan Agricultural University, PR China*

B. HONORS

2019	*Endowed Gordon D Cain Chair Professor, LSU College of Agriculture*
2009	*LSU AgCenter Rogers Research Excellence Award*
2008	*LSU Chapter Sigma Delta Gamma Honor Society Research Award*
2008	*Elected to be an International Academy of Wood Science (IAWS) Fellow*
2007	*Awarded JSPS Fellow, Shizuoka University, Shizuoka, Japan*
2005	*Forest Products Society Markwardt Wood Engineering Award, Madison, WI*
2004	*Endowed Professorship - Roy O Martin Sr. Professor, LSU AgCenter*
1993	*Wood Award, Forest Products Society Madison, WI*

C. POSITIONS HELD

7/2009-present	*Adjunct Professor, LSU Chemistry*
7/2004-present	*Professor, Renewable Natural Resources, LSU AgCenter*
7/2000-6/2004	*Associate Professor, Renewable Natural Resources, LSU AgCenter*
1/1996-6/2000	*Assistant Professor, Renewable Natural Resources, LSU AgCenter*
7/1994-12/1995	*Research Associate, Forestry, Michigan State Univ, East Lansing, MI*
7/1993-6/1994	*Research Associate, Forest Products, Oregon State Univ, Corvallis, OR*
8/1989-6/1993	*Research Assistant, Forest Products, Oregon State Univ, Corvallis, OR*
1987-7/1989	*Research Assistant, Mechanical Engineering, Univ of Tasmania, Australia*

D. SYNERGISTIC ACTIVITIES

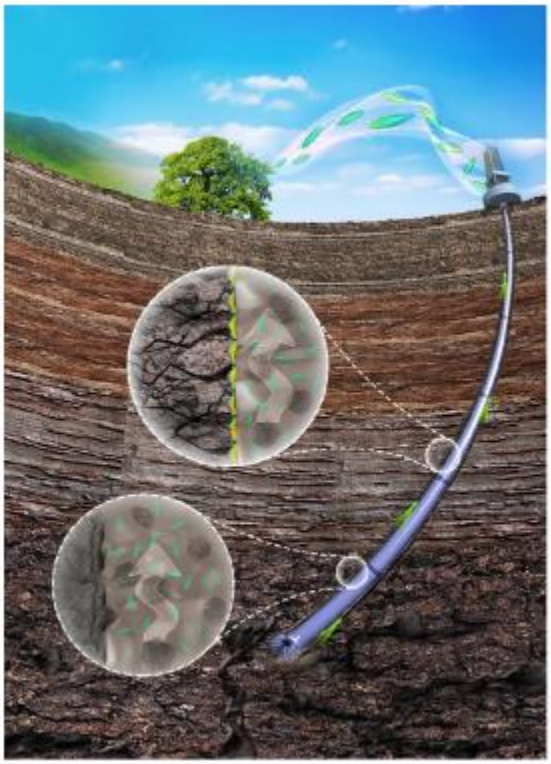
1. *Fellow, EU Academy of Science, International Academy of Wood Science (IAWS)*
2. *Served as Panel Member for NSF SBIR, NSF SIM, USDA 1890 teaching/extension/capacity building; USDA HSI; Chinese NSF, USDA SBIR, and CSREES NRI; and as proposal reviewer for USDA NRI/SBIR/NIFA, Canadian NSRP, Swiss NSF, Chinese NSF*
3. *Member of ISO, FPS, SWST, ACS, AWPA, and IRG;*
4. *Editorial Boards: Cellulose and Wood/Fiber Science; Editor for International Journal of Polymer Science, and reviewer for 20 journals including Science, Advanced Material, Biomacromolecules, Macromolecules, NanoScale, ACS AMI, Cellulose, ACS SCE*

Introduction

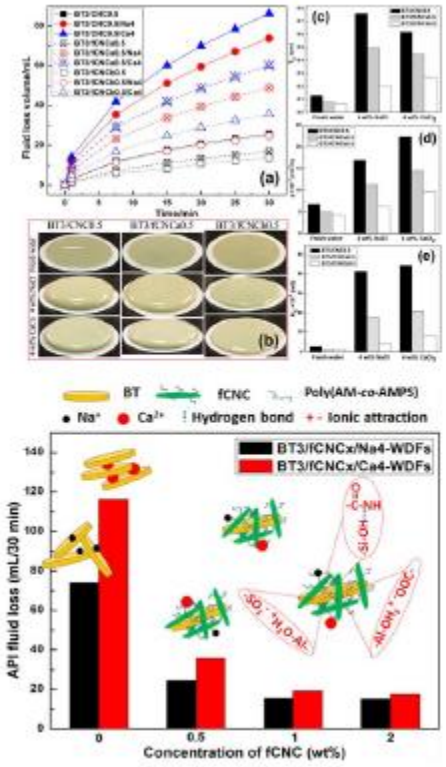
The approaching era of sustainable development and rapid increase in global energy demand necessitate smart, high-performance drilling fluids with sustainability, advanced rheology, superior filtration performance, outstanding thermo- and salt-tolerance, and stimuli responsiveness to make the exploration and production of oil and gas more safe, efficient, productive and environmentally friendly. Herein, advanced water-based drilling fluids (WDFs) composed of bentonite (BT) and biomass-derived cellulose nanocrystals (CNCs) are formulated by taking advantages of gelling and waterproofing capacity of nanoplatelet-like BT and tunable surface chemistry of CNCs. In order to achieve stimuli responsiveness as well as to implement thermo- and salt-resistance into CNC/BT-WDFs, two categories of functionalized CNCs, i.e., themo-thickening CNCs (tCNCs) and salt-resistant CNCs (sCNCs) are rationally designed and synthesized. The formulated tCNC/BT-WDFs exhibit promising temperature tunable rheological performance; demonstrating the controllable suspending and carrying capacity for drill cuttings. The synthesized sCNCs bearing salt-tolerant polymers are attached on the surface of BT platelets, screen their salt-susceptible sites, and hence greatly enhance the salt-resistance of BT-WDFs for filtration performance. This work demonstrates that CNCs can be used as sustainable, smart, and multifunctional agents in water-based nanofluid formulations through rational surface functionalization design, paving the way for their widespread applications in harsh, complex formation excavation.

Li, MC, Wu, Q., Han J, Mei C, Lei T, Lee S., J Gwon. Overcoming Salt Contamination of Bentonite Water-based Drilling Fluids Using Dual-Functionalized Cellulose Nanocrystals. ACS Sustainable Chem. Eng. 2020, 8, 11569−11578.

Abstract: The depletion of onshore oil reserves along with rapid increase in global energy demand have driven oil industry to explore and produce oil from deepwater field. However, due to the high salinity in the subsea formation, salt contamination is becoming one of the most critical challenges to bentonite-water-based drilling fluids (BT-WDFs), causing undesirable changes in the density, rheological and filtration properties. Herein, we reveal the mechanisms of salt contamination in BT-WDFs, and demonstrate the effectiveness of biomass-derived cellulose nanocrystals (CNCs) as anti-salt agents in BT-WDFs through rational dual surface functionalization for the first time. Poly(acrylamide) (PAM) and poly(2-acrylamido-2-methyl-1-propanesulfonic acid) (PAMPS) are grafted on the surface of CNCs through free radical graft polymerization. The dual-functionalized CNCs (fCNCs) are attached onto both face and edge surface of BT platelets, effectively shielding the ion-sensitive sites of BT platelets. At the same time, the highly negatively charged PAMPS grafts on the surface of fCNCs immobilize ions via ionic bond, preventing ions to be attached on the ion-sensitive sites of BT platelets. These dual functions lead to dramatic improvement in the salt-tolerant performance of BT-WDFs. Moreover, the salt-tolerant performance of BT-WDFs can be further tuned by controlling the grafting ratio and concentration of fCNCs. This work demonstrates that CNCs can be used as sustainable and multifunctional agents in BT-WDFs through rational surface functionalization design, paving the way for their application in deepwater reservoir excavation.



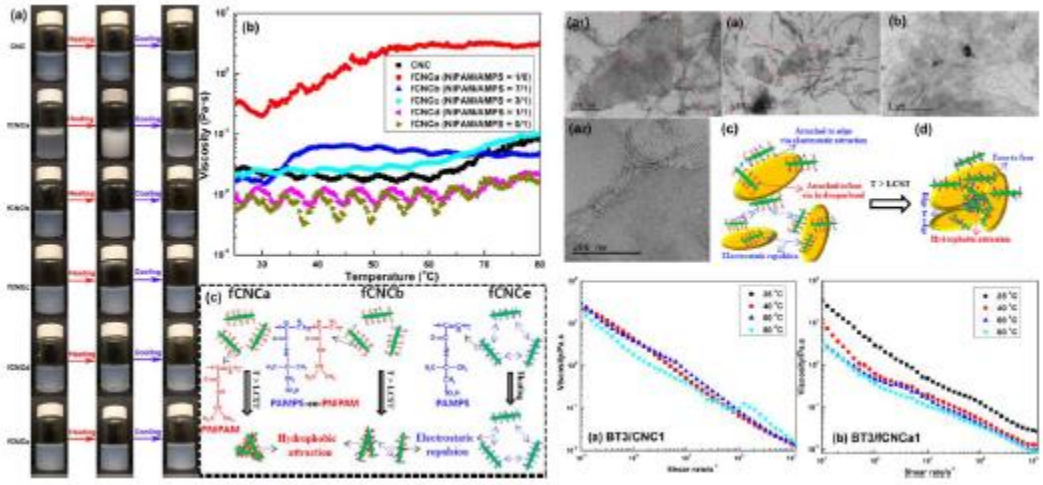
CNM in Drilling Fluid Application



Salt Responsive Fluid Formulation

Li, MC, Wu Q., Lei, T, C Mei, X Xu, S Lee, and J. Gwon. Thermo-Thickening Drilling Fluids Containing Bentonite and Dual-Functionalized Cellulose Nanocrystals. ACS Energy and Fuels, 2020, 34(7):8206-8215.

Abstract: High performance nanocomposites with a homogeneous dispersion of nanoparticle inclusion and phase separated morphology has received a great attention. Cellulose nanocrystals (CNCs) was first grafted with hydrophobic poly(methyl methacrylate)-PMMA chains to produce modified CNCs (PMCNCs) with an increased thermal stability and hydrophobic surface. Such surface tailored CNCs effectively influenced the phase morphology and consequently altered mechanical properties of the poly(butyl acrylate)-co-PMMA (PBA-co-PMMA) nanocomposites. Morphological analysis indicated a nanoscale phase separation behavior of PMCNCs/PBA-co-PMMA nanocomposites with PBA as the soft domain and PMMA as well as CNCs as hard domain. The nanocomposites with 10 wt% PMCNCs/PBA-co-PMMA had an increase in Young's modulus of more than 20-fold and in tensile strength at about 3 times compared to that of neat PBA-co-PMMA copolymer. Therefore, the PMCNCs played a crucial role for controlling their dispersion and tuning the phase morphology of composites. It is of primary importance for such micro-phase separation to delineate potential paths for nano scaled morphological control and to subsequently tune resultant composite properties.



Conclusions

We have demonstrated a new concept of formulating advanced WDFs, including thermo-thickening and salt-resistant WDFs using surface functionalized CNCs to facilitate the advent of sustainable, smart and multifunctional drilling fluid era. tCNCs were synthesized through surface grafting of PAMPS and PNIPAM using APS as an initiator. The thermo-responsive behaviour of tCNCs can be tailored by tuning the feeding molar ratio of NIPAM/AMPS. Due to the attachment of tCNCs on the surface of BT platelets, the presence of negatively charged PAMPS grafts enhanced the electrostatic repulsion among BT platelets, generating the exfoliated structure under room temperature. However, when the temperature exceeded the LCST, the phase transition of PNIPAM grafts on the surface tCNC occurred, leading to the aggregation of tCNCs. This further drove the BT platelets to associate together, inducing the thermo-thickening rheological behaviours. sCNCs were also prepared through surface grafting of PAM and PAMPS using APS as an initiator. It was found that PAM and PAMPS grafts were attached on the surface of BT platelets and effectively shielded their salt-susceptible sites, leading to superior salt-resistance of BT-WDFs. We envision that these findings serve as a crucial step forward toward the development of sustainable, smart, multifunctional nanofluids for drilling complicated formations.

Recent Improvements in Synthetic Organic and Medicinal Chemistry

by James Cook, Member EUAS

Short Biography

Dr. Cook graduated with a PHD in chemistry from the University of Michigan. He has been a leader in the search for safer drugs to treat patients afflicted with different CNS disorders for over thirty years, including anxiety disorders, neuropathic, pain, resistant forms of epilepsy,schizophrenia,Tourette's syndrome, migraine headaches, depression as well as others. He has published 500 papers in synthetic organic chemistry and neuroscience. One of his compounds was licensed to Bristol Myers Sguibb for anxiety disorders(in humans,Phase I) which led to the development of a back up,KRM-II-81,which is very active in models for treatment of pain,is anxiolytic and is a terrific anticonvulsant. He has patented and licensed this compound to RespireRx for epilepsy, as well as neuropathic pain. He has filed over 70 patents.

He cofounded with Marquette University ,Promentis Pharmaceutical Company, which currently has a compound in Phase II for anxiety and obsessive compulsive disorders. He also developed a lead compound for asthma,which Dr Arnold took, improved upon and formed the basis of the MIDD formed start up company ,Pantherics. Very recently he cofounded a company with Dr.Soma Sengupta and Dr.Daniel Krummel from the University of Cincinnati, called Amlal Pharmaceuticals. His group's compounds are active against Group III cancers, including pediatric brain tumors and melanomas. He is currently working on a license with Alpha Cog with Dr. Etienne Sibilli at CAMH for a compound active against depression that is also precognitive. It is the precognitive and antianxiety effect that makes this compound so novel and we expect it will be active against the negative symptoms and cognitive deficits of schizophrenia. This antidepressant,procognitive agent,GL-II-73, is being targeted toward the treatment of depression, schizophrenia, and Alzheimer's Disease.

In our research group we have been interested in replacing Valium,Xanax,and other sedating, addictive benzodiazepine tranquilizers with ones with no side effects. We have developed potential drugs with an imidazodiazepine structure,which is called a "privileged structure". It is a hybrid of two compounds that have been in humans for over 45 years,with a minor structural change,that inhibits activity at alpha 1 receptors in the brain that cause sedation,ataxia,amnesia,addiction and dependence like Valium. Our lead compound KRM-II--81 has proven very effective in 5 animal models of resistance/refractory epilepsy,which should work in children and adults when other drugs do not ,or other drugs do,but put you to sleep, or the patient develops tolerance. Secondly ,the antinociceptive activity of this compound has been carried out in 7 different models and it was more active against pain than the known gabapentin or tramadol(Lilly). We believe the data indicates it should be active against diabetic neuropathy, back pain,fibromyalgia,complex regional pain syndrome, neuropathic pain and cancer pain.In a recent pain model it showed no signs of tolerance(like morphine does),nor dependence, nor was it sedating or ataxic in rhesus monkeys.

Personal Statement

I have directed a university research laboratory for >30 years focused on synthetic organic and medicinal chemistry with a particular interest in compounds that modulate CNS neurotransmission. Research under my direction has resulted in over 450 peer reviewed publications, many of which deal with fundamental and

applied studies on gamma amino butyric acid ion type A ($GABA_A$) channels that comprise the major inhibitory neurotransmitter system in the central nervous system. Alterations of $GABA_A$ function are known to occur in many neurological and psychiatric disorders including neuropathic pain, anxiety, panic disorder, epilepsy, hypersensitive behavior, phobias, schizophrenia, alcoholism, Angleman's syndrome, and Rhett's syndrome, as well as effects that lead to or complicate drug abuse. A currently funded project is to uncover the neurochemical mechanisms underlying these disorders through the design, synthesis, and analysis of novel GABAergic ligands. An example of our progress is the discovery of a series of nonsedating α2/α3 GABAA agonists that are active against neuropathic pain, as well as anxiety disorders and convulsions. These agents do not induce tolerance and are comprised of a non-toxic privileged scaffold (imidazobenzodiazepine). Our patent, PCT published 9/29/2016 WO2016/ 154031A1 forms the backbone of the new startup (Neurocycle Therapeutics) company targeting treatment of epilepsy and pain. Our alcoholism studies are directed at the ability of selected benzodiazepine receptor subtype selective agonists to blunt the discriminative stimulus effects of alcohol, reduce alcohol self-administration and attenuate priming-induced reinstatement of alcohol seeking at doses that do not produce a generalized disruption of behavior or debilitating side effects. For schizophrenia we are developing chiral α5 and α2/α3/α5 GABAergic ligands. Ligands related to our previously characterized compound SH-053-2′F-R-CH3 have been shown to be active in the MAM model of schizophrenia. We currently have developed α3 subtype selective Bz/GABA(A) receptor ligands and are synthesizing them on large scale for animal studies as well as developing more α3 subtype selective ligands. (Namjoshi, et al. *BMC,* 2014). We have been investigating the synthesis of agents active against parasites and microbes for several years, including active against TB, MRSA infections and anthrax (Kabir, Cook et al, BMC,2010) as well as antimalarial, (alkaloids) and antischistosomal agents. Ongoing research in all of these areas includes the synthesis of hundreds of new compounds based on structure-activity-relationship analysis and functional evaluation. The strength of our research is the integration of synthetic organic chemistry with a network of leading experts in neuro-behavioral animal models for each of our disease areas of interest. This systems approach provides an unmatched team for the study of GABAA neurobiology and lead development for future therapeutics. I have considerable expertise designing drug functionality (blood brain barrier transport, bioconversion, metabolism, solubility, formulation) to avoid off-target effects. We have filed over 60 patents, many of which have been issued.

Contributions to Science

1. My early publications outlined the development of rigid ligands that bound tightly (5nM) to the benzodiazepine allosteric site of the Bz/GABA(A) receptor. Because these were rigid ligands, this permitted the generation of the best pharmacophore model of the Bz /GABA(A) α1-6, β3γ2 receptor reported to date. It was used by Neurogen, Merck and J&J to develop pharmacophore models, the latter

of which were later published as their own models that were nearly identical to ours. This work led to an understanding of the difference in the 6 major subtypes, which resulted in the development of XHe-II-053, a nonsedating anxiolytic devoid of side effects. This was patented and licensed to BMS and made it through Phase I clinical trials. It was metabolized to rapidly generate enough efficacy to go into Phase II trials, but it had no toxicity (BMS, unpublished results). This then led to an α2/α3 subtype selective ligand (Hz-166), which is a nonsedating anticonvulsant and anxiolytic, which was licensed to Addiction Theraputix, Inc. Quite recently, this agent has been shown to be active against neuropathic and inflammatory pain. It acts via GABA α2/α3R in the spinal cord and does not develop tolerance. At present, bioisosteres, which have been shown to have a longer duration of action as anxiolytics, demonstrated great PK values and have no sedative activity, are being studied by big pharma under a CDA. Aim—clinical candidates for anxiety disorders, epilepsy and neuropathic pain (Cook et al. PCT WO2016/154031A1(9/29/16)).

a. Huang, Q.; He, X.; Ma, C.; Liu, R,; Yu, R.; McKernan, R.; Wenger, G.; Dayer, C.; Cook, J.M. Pharmacophore receptor models for $GABA_A$/BzR subtypes α1β3γ2, α5β3γ2, and α6β3γ2 via a comprehensive ligand-mapping approach. J. Med. Chem **43**, 71-95 (2000).

b. Paul, J.; Yevenes, G.; Benke, D.; DiLiom, A.; Ralvenius, W.; Witschi, R.; Scheuer, L; Cook, J.M.; Rudolph, R.; Fritsch, J.; Zeilhofer, H., Antihyperalgesia by α2-GABA(A) receptors occurs via genuine spinal action and does not involve supraspinal sites, Neuropsychopharmacology, **39**, 497-487 (2014). PMCID: PMC3870792.

c. Clayton, T.; Poe, M.; Rallapalli, S.; Biawat, P.; Savic, M.; Rowlett, J. Gallows, G., Emala, C.; Kaczorowski, C.; Stafford, D.; Arnold, L.; Cook, J.M.; A Review of the Updated Pharmacophore for the Alpha 5 GABA(A) Benzodiazepine Receptor Model, International Journal of Medicinal Chemistry, vol. 2015, Article ID 430248, 54 pages, 2015. doi:10.1155/2015/430248). PMCID: PMC4657098.

d. Lewter, L.; Fisher, J.; Siemian, J.; Methuku, K..; Poe, M.; Cook, J.M.; Li, Jun-Xu, Antinociceptive Effects of a Novel α2/α3 Subtype Selective GABA(A) Receptor Positive Allosteric Modulator, ACS *Chem Neurosci*, DOI: 10.1021/acschemneur.6b00447 (2017).

2. Based on our α5 pharmacophore Bz/GABA(A) receptor model, we have designed α5β3γ2 receptor agonists that are active in models of schizophrenia (SH-053-2'F-RCH_3) and MDD (mood disorders). Moreover, we showed early in 2014 that if you treat rats with a known antipsychotic for 6 months and then with SH-053-2'F-RCH_3, the ligand has no effect. This clearly shows that patients that have been treated for long periods of time with antipsychotics; their brains are rewired. This explains the failure in phase III of Lilly's drug for schizophrenia. This has also prompted a study into the cysteine/cystine antiporter in regard to glutamate. The studies of ligands in this project led us to cofound with Dr. David Baker, Prementis Pharmaceutical Co., a startup directed toward agents to treat schizophrenia and drug abuse, resulting in 11 patents that have been filed and many issued. Recently

Promentis received 26 million in series C. financing to file an IND and go into phase I.

a. Gill, K.; Lodge, D.; Cook, J.; Ava, S.; Grace, A., A novel α5 GABA(A)R-positive allosteric modulator reverses hyperactivation of the dopamine system in the MAM model of schizophrenia, *Neurospychopharmacology*, **36** 1903-1911 (2011). PMCID: PMC3154109.

b. Gill, K.; Cook, J.; Poe, M.; Grace, A.; Prior antipsychotic drug treatment prevents response to novel antipsychotic agents in MAM model of schizophrenia, *Schizophrenia Bulletin* **40** 341-350 (2014). PMCID: PMC3932102.

c. Cook, J.; Baker, D.; Johnson II, E.M.; Yin, W.; Verma, R., US Application No 14/148959, CIP Application Pub No. US01554410A1, June 5,2014. Notice of Allowance, 2014, 13/465383.

d. Botta, P.; Demmou, L.; Xu, C.; Lu, T.; Poe, M.M.; Xu, L.; Cook, J.M.; Rudolph, u.; Sah, P.; Luth, A.; Regulating anxiety with extra-synaptic inhibition, *Nature Neuroscience*, 18, 1493-1499 (2015). PMCID: PMC4607767.

3. Based on the pharmacophore models of the α4 and α5 subtypes, we developed α4 subtype-selective ligands that are effective in relaxing bronchial smooth muscle and epithelial cells in the lung as a safer alternative to treat asthma. This is in collaboration with Charles Emala, George Gallos, and with colleagues at Columbia University, Stafford and Arnold at UWM. The α4 ligands do not have activity at α1, α2 α3 and α5 subtypes, consequently, there is no fear of CNS activity; these are benzodiazepine-insensitive (site) ligands. The α5 ligands are also active against asthma models and will hydrolyze in the lung or blood (aerosol) after use and be excreted as the acid or glucuronide; will not go through the BBB.

a. Cook, J., Zhou, H., Huang, S., Sarma, P. Zhang, C. Stereospecific Anxiolytic and Anticonvulsant Agents with Reduced Muscle-Relaxant, Sedative-Hypnotic and Ataxic Effects, US Patent Pub. No. **US2010/0004226A1**. Published 1/7/2010.

b. Gallos, G.; Yin, P.; Chang, S.; Zhang, Y.: Xu, D.; Cook, J.M.; Gerthhoffer, W.; Emala, Sr, C., Targeting the restricted α4 subunit repertoire of airway smooth muscle GABA(A) receptors augment airway smooth muschle relaxation. Am. J. Physiol. Lung Cell Mol. Physiol., **302** 248-256 (2012). PMCID: PMC3349365.

c. Stafford, D., Cook, J., Emala, C., Gallos, G., Stephen, M., Arnold, A., Jahan,R., Novel GABA Agonists and Methods of Using to Control Airway Hyperresponsiveness and Inflammation in Asthma. Patent Pub. Nos. **US2013/060859**, **WO2014/047413**, published March 27, 2014.

d. Gallos, G; Yocum, G.; Siviski, M.; Yim, P.; Wen Fu, X.; Poe, M.; Cook, J,; Harrison, N; Perez-Zoghbi, J.; Emala, Sr., C., C., Selective targeting of the α5 subunit of GABA(A) receptors relaxes airway smooth muscle and inhibits cellular calcium handling, Am. J. Physiol. Lung. Cell Mol. Physiol. Doi: 10.1152/ajplung.00107.2014 (2015). PMCID: PMC4421780.

4. We developed the first subtype selective ligand for α6β3γ2 Bz/GABA(A) receptors reported to date. It has no efficacy at benzadiazepine-sensititive subtypes in rodents. Savic, Cook et al., showed it was devoid of sedation, ataxia and amnesia

for it has zero affinity at the alp1 subtypes. Chou, Poe, Cook, et al., have shown it antagonized PCP induced effects on prepulse inhibition (unpublished). There are several α6 subtype ligands that exert even better selectivity. These are being investigated (since α6 subtypes are found exclusively in the cerebral granular layer and olefactory bulb) for treatment of Tourette syndrome, myofascial spasms, OCD and other tic related diseases.

a. Varagic, Z.; Ramerstorfer, J.; Huang, S.; Rallapilli, S.; Sarto-Jackson, I.; Cook, J.; Sicghert, W.; Ernst, M., Subtype selectivity of α and γ site ligands of GABA(A) receptors: Iedntification of the first highly selective positive modulator at α6β2/3γ2 receptors. Bri. J. Pharmacol., **169**,384-399 (2013); PCT Patent Pub No WO2016/19696/A1(12/8/16).

5. The clinical need for novel bronchodialtors for the treatment of bronchoconstrictve diseases remains a major medical issue in asthma and COPD, as well as during some surgeries. Using our α5β3γ2 Bz/GABA(A) subtype selective PAM (SH-053-2^{l}F-RCH$_3$), we showed that targeting of α5 GABA(A) alpha subunits in airway smooth muscle was characteristic of electrophysiological changes indicative of GABA(A) receptor activation that can activate β-agonist mediated relaxation. 2) That GABA(A) α5 receptor activation can directly and spontaneously relax precontracted airway smooth muscle, and that 3) a component of the mechanism involves an attenuation of Ca^{2+} handling as reductions in both Ca^{2+} entry (SOCE) in human airway smooth muscle cells, as well as calcium oscillations in ASM within peripheral lung slices. Selective targeting of the α5 Bz/GABA(A) subunits in lung tissue on ASM represents a new method to treat asthma, etc.

Alleviation of Multiple Asthmatic Pathologic Features with Orally Available and Subtype Selective GABAA Receptor Modulators", Forkuo, G.S.; Nieman, A.N.; Yuan, N.; Kodali, R.; Yu, O.B.; Zahn, N.M.; Jahan, R.; Li, G.; Stephen, M.R.; Guthrie, M.L.; Poe, M.M.; Hartzler, B.; Harris,T.W.; Yocum, G.T.; Emala, C.; Steeber, D.; Stafford, D.C.; Cook, J.M.; Arnold, L.A., *Molecular Pharmaceutics*, (2017), DOI: 10.1021/acs.molpharmaceut.7b00183. PMCID: PMC5497587.

Theories and Methods of Fire Prevention for New Energies

by Jinhua Sun, Member EUAS

Short Biography

Education and Positions

2019~ Chairman, Sub-Committee on Fire Science, University of Science & Technology of China
2004~2019 Vice Director of State Key Laboratory of Fire Science of China, CHINA
2014~ Director of Energy Fire Safety Institute, SKLFS, CHINA
2002~ Professor, University of Science & Technology of China, CHINA
1999~2002 Research Professor, Japan Science and Technology Agency, JAPAN
1996~1999 Ph.D., The University of Tokyo, JAPAN
1988~1996 Associate Professor, Anhui University of Science & Technology, CHINA
1986~1988 M. Sc., Nanjing University of Science and Technology, CHINA
1983~1986 Assistant Professor, Anhui University of Science & Technology, CHINA
1979~1983 B. Sc., Nanjing University of Science and Technology, CHINA

Professional Activities

Vice-Presidents of Asia-Oceania Association for Fire Science and Technology (2007~2020)
Committee Member of the International Association for Fire Safety Science (2008~2017)
Committee Member of the National Science and Technology Award (2010~)
Vice-chairman of Chemical Safety Committee, CIESC (2017~)
Vice-chairman of Building Fire Protection Committee, CFPA (2008~)
Experts of the first national emergency response expert group for work safety (2015~)
Experts of the fifth national work safety expert group (2014~)
Academic Committee Member of University of Science and Technology of China (2009~)
Safety expert committee Anhui Province, Civil blasting group leader (2009~)
Member of Science and Technology Award Committee, Ministry of Public Security (2007~)
Member of Academic Committee of urban safety and disaster prevention, Urban Planning Society of China (2005~2015)
Evaluation expert in international scientific and technological cooperation program, Ministry of Science and Technology of China (2005~)
Executive director of Anhui Fire Protection Association (2005~)
Associate Editorial or Editorial Board of five International Journals (2010~)
Editorial Board of nine national Journals (2003~)
Academic Committee Member of China Fire Protection Association (2003~)

Honors and Awards

National Science and Technology Progress Award, First-class Award, China (1993)
Member of Hundred Talent Program, Chinese Academy of Sciences (2001)

Outstanding Member Hundred Talent Program, Chinese Academy of Sciences (2005)
National Science and Technology Progress Award, Second-class Award, China (2006)
Science and Technology Award for Young Scientist, Anhui Province (2006)
Safety Science and Technology Award of State Administration of Work Safety, Second-class Award (2006)
Beijing Science and Technology Award, Third-class Award, Beijing (2008)
Teaching Award of Anhui Province, First-class Award, Anhui Province (2010)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2014)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2014)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2017)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2017)
Science and Technology Innovation Award, First-class Award, China Fire Protection Association (2018)
Science and Technology Progress Award, First-class Award, China Highway and Transportation Society (2018)
Special government allowance of the State Council（2019）

Professor Sun Jinhua has long been devoted to academic research and education in the area of fire science and fire protection. He has made substantial accomplishments in a number of fields in fire safety science and engineering, including fire risk assessment, performance-based fire protection design, building fire safety, industrial fire safety, fire safety in new energies. He led as a PI more than 20 important national research projects, such as the National "973 Program", key projects funded by National Natural Science Foundation of China (NSFC), the "11th Five-Year plan" and the "13th Five-Year Plan" national key R&D program, the sixth Framework Project of the EU International Cooperation Program in Science and Technology, NSFC general projects, and "Outstanding Talents" project funded by the Chinese Academy of Sciences.

Prof. Sun has published more than 350 papers in peer-reviewed journals, including Progress in Energy and Combustion Science, Combustion and Flame, Renewable and Sustainable Energy Reviews, et al, which have been cited more than 7,400 times (Web of Science). Contributions have also been recorded in 11 academic books or book chapters and over 40 keynote or invited talks at national or international conferences. In addition, Dr. Jiang has supervised more than 40 PhD students.

Major Research Areas

1. Theories and methods of fire prevention for new energies
2. Methods for fire risk assessment and safety design of buildings and urban areas
3. Theory of fire dynamics, fire prevention and control for buildings
4. Industry fire dynamics and fire prevention

Selected Publications in 2020

1. **Qi Sun, Lin Jiang, Mi Li, Jinhua Sun∗, Assessment on thermal hazards of reactive chemicals in industry: State of the Art and perspectives, Progress in Energy and Combustion Science 78 (2020) 100832**

Thermal hazards of reactive chemicals have been a major concern due to the unceasing occurrences of fire and explosion accidents in industry. Understanding thermal threats of

these chemicals not only contributes to the process safety and sustainability in the research and development (R&D) level, but promotes the efficiency of loss prevention, firefighting and emergency responses. Numerous studies have been conducted towards the comprehensive assessment of thermal hazards of reactive chemicals. The chemicals and methods varied in these studies, and yet some topics were commonly concerned by researchers in relevant fields. Further to say, these topics should also be targeted at when dealing with thermal hazards of new chemicals in future. This article provides an up-to-date overview of the common ground regarding the comprehensive understanding of thermal hazards of reactive chemicals in industry level; whereby, the main limitations and challenges to be faced are explored. The discussed key points include, the classification and reactivity of typical reactive chemicals, the fundamental steps towards the comprehensive understanding of their thermal hazards (including the identification of reaction mechanisms, the calculation of reaction kinetics and thermodynamics, and the characterization of thermal safety properties), and the applicable theoretical, experimental and engineering approaches in each step. The primary goal of this review is to lay out the essential basics that should be focused in every trial to comprehensively understand the thermal hazards of reactive chemicals. The further research directions are also presented based on the current research gaps and the context of Industry 4.0.

2. **Huiqi Cao, Qiangling Duan, Hua Chai, Xiaoxi Li, Jinhua Sun∗, Experimental study of the effect of typical halides on pyrolysis of ammonium nitrate using model reconstruction, Journal of Hazardous Materials 384 (2020) 121297**

The energetic material ammonium nitrate (AN) is used as an industrial raw material; however, it presents a pyrolysis and explosion hazard during transportation and storage, especially when mixed with impurities. To study the effects of typical halides on the thermal decomposition kinetics of AN, a series of precision thermogravimetric analysis experiments at four heating rates were carried out in a nitrogen atmosphere. Based on derivative thermogravimetric analysis, the addition of sodium halides was found to change the kinetic reaction mechanism of AN pyrolysis. The activation energies were obtained using the isoconversional method, and the pre-exponential factor was derived from the kinetic compensation effect. Models of the kinetic reaction mechanism were reliably reconstructed by combining composite kinetic data processing methods, namely, modelfree method, model-fitting method, and parameter simulation. A comprehensive analysis showed that the addition of sodium halides shifts the kinetic mechanism of the pyrolysis of AN toward different dominant reaction models (such as reaction order models, power law models, or phase boundary control models) than those of the original reaction model. The results are helpful as a reference and provide guidance for the determination of AN pyrolysis behavior and the simulation of parameters.

3. **Qian Zeng, Qiangling Duan, Dongxu Sun, Ping Li, Mengyuan Zhu, Qingsong Wang, Jinhua Sun∗, Experimental study of methane addition effect on shock wave propagation, self-ignition and flame development during high-pressure hydrogen sudden discharge from a tube, Fuel 277 (2020) 118217**

In this paper, experimental investigations are carried out to study the effects of methane addition (2.5%, 5% and 7.5% vol.) on self-ignition and subsequent flame propagation of pressurized hydrogen release via a tube. The visualization method utilizing the high-speed

direct photography and the measurements of pressure and light sensors are applied in this study. The result shows that the existence of methane can reduce the shock wave overpressure and the temperature of shock-heated air. Therefore, it has great effects on the self-ignition possibility. The minimum burst pressure required for self-ignition increases from 2.89 MPa (0% CH4) up to 6.05 MPa (7.5% CH4). Besides, methane addition can extremely reduce flame intensity and inhibit flame development inside the tube. Three possible self-ignition mechanisms for the hydrogen with methane addition are discussed. Under the effects of methane addition, hydrogen flame spouting from tube exit tends to blow out. In all cases with 7.5% methane addition, no self-sustained jet flame is formed outside the tube for burst pressure up to 10.0 MPa. When self-sustained flame is formed in a confined space, a great rise in overpressure is generated due to the intense combustion. It is suggested that more methane addition can reduce the self-ignition probability and the formation of self-sustained flame. However, with the increasing of CH4 additions, once the jet fire is formed in a confined space, it may cause greater overpressure and thus bring greater casualties and property losses.

4. **Wenxin Mei , Lin Zhang , Jinhua Sun , Qingsong Wang*, Experimental and numerical methods to investigate the overcharge caused lithium plating for lithium ion battery, Energy Storage Materials 32 (2020) 91–104**

Lithium plating can threaten the lithium-ion battery safety, which can be caused by overcharging. Detection on lithium plating is of vital importance in battery management system (BMS). Both experimental and numerical methods are involved in detecting overcharge caused lithium plating for a commercial 26650 type LiNi1/3Co1/ 3Mn1/3 (NCM)/Graphite cell within this work. Differential analyses are conducted to monitor the lithium stripping capacity and voltage, topography observation also provides a strong basis for lithium plating detection. A deeper detection on lithium plating is conducted by numerical model, which is validated by experiment at several cases. Lithium plating first occurs at the anode-separator interface, if it continues to proceed until the current collector-anode interface, complete lithium plating is appeared. While if lithium plating cannot proceed to the current collector-anode interface, but somewhere before the negative current collector, incomplete lithium plating is considered. The depth of lithium plating (DLP) is defined to quantify the degree of incomplete lithium plating, indicating that incomplete lithium plating can be occurred at the overcharge voltage range of 4.5–4.586 V. Besides, good linear relationships between lithium plating time and capacity with overcharge voltage are observed at 0.2 C and 0.5 C. Further consideration results in alleviating lithium plating by increasing the anode thickness with the reasonable N/P ratio. It is discovered that 6.57% anode thickness excess with slight overcharge before 4.6 V can effectively shorten plating time and achieve “complete non-lithium plating”.

Affective Computing and Intelligent Robot, Natural Language Processing, Artificial Intelligence, Language Understanding - Communication & Information Retrieval

by Fuji Ren, Member EUAS

Short Biography

Prof. Fuji Ren received his B.E. and M.E. degrees from Beijing University of Posts and Telecommunications, Beijing, China, in 1982 and 1985, respectively. He received his Ph.D. degree in 1991 from Hokkaido University, Japan. He is a professor in the Faculty of Engineering of Tokushima University, Japan. His research interests include information science, artificial intelligence, language understanding and communication, affective computing, and Intelligent robot. He is a member of The Engineering Academy of Japan, a fellow of IEICE and CAAI. He is a fellow member of the Japan Federation of Engineering Societies. He is the president of the International Advanced Information Institute. He is the author/co-author/editor of eight books and over 500 research publications.

Dr. Fuji Ren is currently the Professor and Director of Affective Computing and Intelligent Robot Laboratory in Tokushima University. He is also the President of International Advanced Information Institute in Japan. He is a member of The Engineering Academy of Japan, a member of EU Academy of Sciences, a fellow of the Japan Federation of Engineering Societies, a fellow of The Institute of Electronics, Information and Communication Engineers, and a fellow of Chinese Association for Artificial Intelligence.

He received his B.E. degree in 1982 and M.E. degree in 1985 from the department of Computer Science, Beijing University of Posts and Telecommunications, Beijing, China. He received his Ph.D. in 1991 from Faculty of Engineering, Hokkaido University, Sapporo, Japan. From 1991 to 1994, he worked at CSK in Tokyo, Japan where he was the chief NLP researcher. He joined the Faculty of Information Sciences at Hiroshima City University as an Associate Professor in 1994. In 2001, he became a Professor in the Faculty of Engineering at Tokushima University. He has been the president of AIA International Advanced Information Institute since 2003. He serves as the Director of the Dept. of

Information Science and Intelligent Systems from 2006 to 2010, the vice Dean of Information Solution Branch of Graduate School of Engineering from 2010 to 2012, and Dean of Information Solution Branch Graduate School of Engineering from 2012 to 2016 at Tokushima University.

He also holds professor positions at Dalian University of Technology, Harbin University of Technology and Xi'an Jiaotong University. He holds the roles of Advisory Professor at Beijing University of Posts and Telecommunications, Research Advisor at Tsinghua University, Visiting Professor at University of Science and Technology of China, Yangtze River Professor at Nanjing University, and Advisory Professor at Tongji University. He was a visiting professor at CRL (Computing Research Laboratory) at New Mexico State University, a visiting research professor in the College of Engineering, at Florida International University, and a visiting professor in Harvard University in the USA.

His current research interests include Affective Computing and Intelligent Robot, Natural Language Processing, Artificial Intelligence, Language Understanding and Communication, Information Retrieval, Super-Function Methodology, Machine Learning, Knowledge Engineering, and Enlarged Health and Intelligence Education.

He has made fundamental contributions in the fields of human emotion recognition and robotic emotion creation, as well as natural speech understanding and emotional robotics development. He was the first in the world to propose the theory of mental state transition network, which established a methodology for recognizing human emotions, creating machine emotions, and constructing large emotional corpuses. In addition, he researched and developed fundamental technologies for the development of robotic brains and emotions based on language, speech, and facial expressions.

He has directed and participated in over 50 research and development projects, as the PI of more than 30 grants with over 500 million Yen in total funding.

He has authored or co-authored more than 20 books, 300 research journal papers and 500 conference papers. Many of his publications appeared in top conferences and journals, including IEEE, ACM, IEICE, IEEJ, CAAI and Information Sciences. He has been invited as a speaker or keynote speaker for more than 100 times in the USA, China, Japan, Singapore, France, and other countries.
(Please see http://pub2.db.tokushima-u.ac.jp/ERD/person/19966/work-en.html for the list.)

He has supervised 42 Ph.D. students (list of Ph.D. supervised by Prof. Fuji Ren) and more than 130 Masters students.

He received more than 50 Awards and Honors, such as The Chinese Government Friendship Award, PRC, 2019; Outstanding Contribution Award for the 7th Council

of the Chinese Association for Artificial Intelligence, CAAI, 2019; Academician of The Engineering Academy of Japan, 2018; Academician of EU Academy of Sciences, 2018; Invention Prize, for "Multi-modal emotional computing and advanced intelligent applications", China Association of Inventions, 2018; Science and Technology Award (Science and Technology Promotion Category), Tokushima Prefecture, Japan, 2018; Wu Wenjun Artificial Intelligence Science and Technology Progress Award, China, 2018; Fellow of The Institute of Electronics, Information and Communication Engineers, Japan, 2017; Fellow of The Chinese Association for Artificial Intelligence, China, 2017; Best Paper Award, for the paper entitled "Learning Efficient Drawing Sequence Through Training of Recurrent Neural Network Model", CAAI and IEEE, 2017; Korakukai Foundation Award, for "To create an evolutionary advanced intelligent robot which have a brain and mind", Japan, 2016; Industry-University-Research Cooperation Innovation Award, China Industry-University-Research Institute Collaboration Association, China, 2016; Best Paper Award, for the paper entitled "Text classification based on word co-occurrence with background knowledge", CAAI, 2016; Outstanding Contribution Award, Scientific Chinese Person of the Year, China, 2016; Engineering Festival 2015 Excellence Award, for "Development of emotional development robot capable of rich emotional expression and recognition", Japan, 2015; Wu Wenjun Artificial Intelligence Science and Technology Award, for "Advanced Interactive Robot based on Advanced Intelligence", Association for Artificial Intelligence, 2014; Best Paper Award, for the paper titled "Class-indexing: The Effectiveness of Class-Space-Density in high and Low-Dimensional Vector Space for Text Classification", IEEE, 2012; Fellow of Japan Federation of Engineering Society, Japan, 2009; Yangtze River Scholar, the highest academic award issued to an individual in higher education by the Ministry of Education of PRC, 2006; 12th Gennai Award for Natural Science Award, Japan, 2005, etc.

He served at more than 200 international conferences as chair, steering committee member, advisory committee member, executive committee member, program committee member, and organizing committee member at meetings of IEEE, CAAI, IEICE, IASTED, IJAI and other organizations. These include Founder and General Chair of the International Conference on Natural Language Processing and Knowledge Engineering, IEEE, CAAI (2003- present); Steering Committee Co-Chair, The 10th International Workshop on Assistive Engineering and Information Technology (AEIT 2020); General Co-Chair, the 4th Asian Conference on Artificial Intelligence Technology, (2019- present); Program Committee Co-Chairs, THE 3rd China Intelligence Education Conference (2019- present); Publicity Co-Chair of 14th IEEE International Conference on Networking, Sensing and Control, (2017-2018); Program Committee Co-Chairs, IEEE International Conference on Cloud Computing and Intelligence Systems, (2011- present); Advisory Board, The 9th International Conference on Rough Sets and Knowledge Technology (RSKT 2014-2014); Steering Committee, International Workshop on Assistive Engineering (2013- present); General Co-Chair, 2011 International Conference on Information Theory and Information Security (2010-2011); General Chair, International

Conference on Advanced Intelligence and Global Engineering Education (2008-2015); Program Committee Co-Chair, 2010 Multi-Conference on Advanced Intelligence (2010-2011); International Advisory Board Chair, 2009 International Conference on Information Management, Innovation Management and Industrial Engineering,(2009-2009); Organizing Committee Co-Chair, International Conference on Information,(2001-2009); International Advisory Board Chairs, International Conference on Advanced Intelligence (2008-2012); The General Chair, International Symposium on Artificial Intelligence and Affective Computing, (2006-2010); and Program Chair, Joint Workshop on Intelligent System and Information Processing (2016-2017).

He served as editor-in-chief, area editor-in-chief, and editor on more than 20 academic journals, including editor-in-chief, International Journal of Advanced Intelligence, (2009–present); editorial board, CAAI Transactions on Intelligent System, (2013–present); editorial board, Enterprise Information Systems, (2012–present); editorial board, Research Journal on Computer science and computer engineering with applications, (2010– present); editorial board, The Journal of China Universities of Posts and Telecommunications, (2006– present); editorial board, Science & Technology Review, (2006– present); editor, Journal of Chinese Information Processing, (2005-present); editor, Journal of Beijing University of Posts and Telecommunications, (2006– present); associate editor, International Journal of Innovative Computing, Information and Control, (2005– present); editor, International Journal of Information Acquisition, (2005– present); associate editor, Asian Information-Science-Life, (2002– 2004); editor, International Journal of Information Technology and Decision Making, (2004– present); area editor-in-chief, International Journal of Information, (1998– present); editor, International Journal COLIPS, (1996-2005); editor-in- chief, Journal of Science and Technology, (1995-1998); editorial board member, Electronics, and others.

He was invited to be a senior overseas consultant for the BUPT (Beijing University of Posts and Telecommunications) Academic Committee, a consultant for the Beijing Lab. of Multi-Media, a senior consultant for Japan PtoPA Inc. and AGI Inc., an academic committee member of the Chinese national laboratory of pattern recognition, an overseas assessor of the Chinese Academy of Sciences, and a senior overseas consultant of China Council for the Promotion of Applied Technology Exchanges with Foreign Countries. He is Honorary Vice President of Chinese Association for Artificial Intelligence, (2019-present); Vice President of Chinese Association for Artificial Intelligence, (2010-2019); Member of Human Resources Development Committee of EAJ, Japan, (2018-present); President of The Association for Chinese Scientists in Japan, (1993-1995); President of Chinese Academy of Science and Engineering in Japan, (2001-2005); Honorary President of Chinese Academy of Science and Engineering in Japan, (2006-present), and others.

Asymmetric Catalysis for C-C Bond Formation by Chiral Lewis and Brønsted Acids

by Hisashi Yamamoto, Member EUAS

Short Biography

Education

B. S.	*Kyoto University, 1967 (Prof. H. Nozaki, Thesis Director)*
Ph. D.	*Harvard University, 1971 (Prof. E. J. Corey, Thesis Director)*

Professional:

1971-1972	*Researcher, Toray Industries, Inc. (Prof. J. Tsuji, Adviser)*
1972-1976	*Instructor, Kyoto University (Prof. H. Nozaki, Adviser)*
1976-1977	*Lecturer, Kyoto University*
1977-1980	*Associate Professor, University of Hawaii*
1980-1983	*Associate Professor, Nagoya University*
1983-2002	*Professor, Nagoya University*
2003-	*Professor Emeritus, Nagoya University*
2002-2012	*Professor, The University of Chicago*
2012-	*Professor Emeritus, The University of Chicago*
2012-	*Professor and Director of Molecular Catalyst Research Center, Chubu University*
2012-	*Research Supervisor, JST Crest Project of Molecular Technology*
2014-	*Research Supervisor, JST-ANR Joint Project of Molecular Technology*
2016-2018	*President of Chemical Society of Japan*

Hisashi Yamamoto is an internationally recognized scholar whose contributions to organic chemistry span a wide range: from articulating and demonstrating new concepts of designer acid catalysis, to elucidating the stereochemical foundations of organic reactions, and to the creative invention of powerful new synthetic methods and their applications including for his new catalytic peptide synthesis. His distinctive contributions to all of these endeavors are characterized by originality and creativity. The breadth of his research accomplishments reflects an intellectual virtuosity in the application of chemical principles to important synthetic and mechanistic problems. His most important contributions are summarized below, highlighting both the scope and depth of his accomplishments over the past 45 years. Most noteworthy of these numerous achievements are the novel aspects of Lewis and Brønsted acid catalysts he has brought to light in selective organic synthesis since the 1970s. During his career, he has discovered a wide variety of powerful new synthetic reactions, reagents, and catalysts based on acid catalysis. Through his dedicated efforts, Lewis and Brønsted acids are now recognized as major tools in the synthesis of both simple and complex organic molecules. Among Yamamoto's many superb contributions, the following are especially worthy of mention.

Yamamoto has published over 550 papers and over 145 reviews, which have been cited more than 30,000 times (50,000 including books), with an h-index of 96 (113 by Google).

His contributions have been recognized by his being a recipient of, among others, the Prelog Medal (1993), the Chemical Society of Japan Award (1995), Le Grand Prix de la Fondation Maison de la Chimie (2002), the National Prize of Purple Medal (Japan) (2002), the Tetrahedron Prize for Creativity in Organic Chemistry (2006), the Japan Academy Award (2007), the Grand Prize of the Synthetic Organic Chemistry of Japan (2009), the ACS Award for Creative Work in Synthetic Organic Chemistry (2009), Fellow of Amer. Academy Arts and Science (2011), the Noyori Prize (2011), the Fujiwara Prize (2012), and the Roger Adams Award (2017) which is the highest award for organic chemistry in the US, Orders of the Sacred Treasure, 2018, The Person of Cultural Merit, 2018, Barluenga Lectur. medal, 2018, Member of EU Academy of Sciences, 2019.

Hisashi Yamamoto is an internationally recognized scholar whose contributions to organic chemistry span a wide range: from articulating and demonstrating new concepts of acid catalysis in organic synthesis, to elucidating the stereochemical foundations of organic reactions, and to the creative invention of powerful new synthetic methods and their applications. His distinctive contributions to all of these endeavors are characterized by originality and creativity. The breadth of his research accomplishments reflects an intellectual virtuosity in the application of his original chemical principles to important synthetic and mechanistic problems. His significant contributions are summarized below, highlighting both the scope and depth of his accomplishments over the past 50 years. Most noteworthy of these numerous achievements are the novel aspects of Lewis and Brønsted acid catalysts he has brought to light in selective organic synthesis since the 1970s. During his career, he has discovered a wide variety of powerful new synthetic reactions, reagents, and catalysts based on acid catalysis. Through his dedicated efforts, Lewis and Brønsted acids are now recognized as major tools in the synthesis of both simple and complex organic molecules. Among Yamamoto's many superb contributions, the following are especially worthy of mention.

Asymmetric Catalysis for C-C Bond Formation by Chiral Lewis and Brønsted Acids

In what is likely to become his most significant chemical legacy, Yamamoto has formulated a new paradigm for the chiral catalysis of reactions of main group elements by demonstrating chiral Lewis and Brønsted acid-catalyzed asymmetric processes. In the early 1980s, he first introduced chiral binaphthol as a key ligand for chiral Lewis acid catalysts. This work was the forerunner of a vast quantity of present-day research on C_2 symmetry-based chiral Lewis acid catalysts, now known as privileged ligands but originated by him. Based on his knowledge of organoaluminum chemistry, he designed an organoaluminum catalyst using 3,3'-disubstituted binaphthol for the first asymmetric hetero-Diels-Alder reaction in 1988. It was his Brønsted /Lewis acid combined system, which offered him a unique opportunity, as this produced the most efficient asymmetric carbon-carbon formations based on a Lewis acid catalyst. Over thirty years ago, his discovery of a tartaric acid-based catalyst (CAB catalyst) and an amino acid-based catalyst (oxaborolidine-type catalyst) led to the first and the most general enantioselective Diels-Alder reaction of a broad range of dienes and dienophiles. This catalyst was indeed shown to be the first efficient catalyst for asymmetric aldol, ene, and allylation reactions. His silver-catalyzed aldol and allylation process has provided a new entry into the creation of a quaternary carbon stereogenic center for asymmetric synthesis. A similar concept was employed for his catalytic asymmetric protonation, which is capable of creating a long-sought chiral proton that induces the first asymmetric and biomimetic polyene cyclization. The use of 8-hydroxyquinole-based chiral Lewis acid catalysis was a recent contribution of his to acid catalysis. The catalyst is designed as a rigid metal complex of "the *cis*-β configuration", which makes the metal center of "C_1 chirality". The ligand turned out to be a brand new privileged ligand for asymmetric synthesis; catalytic asymmetric pinacol coupling, NH reaction, Mukaiyama-Michael addition, Pudovik reaction, Strecker reaction, hydrocyanation, Nagata-Michael addition, and nitroso Diels-Alder reaction with complete enantiocontrol. In fact, most of the asymmetric carbon-carbon bond-formation processes recognized today are based on Yamamoto's early discoveries. Yamamoto published a very important paper in 2015, which reported a catalyst of two independent metal systems. Two metals are independent of each other: one metal holds the substrate and the other metal is

responsible for the desired reaction at an isolated position. This enzyme like catalyst using two independent metal centers is responsible for effective asymmetric epoxidation, sulfoxidation, and N-oxide formation otherwise unaccomplished.

Even more recently, he designed several chiral Brønsted acid catalysts with high reactivity for various asymmetric transformations. The original Akiyama-Terada catalyst is effective for nitrogen containing molecules. However, his phosphoramide catalyst can activate oxygen-containing molecules and greatly expand the utility of the catalyst up to 99%ee. This field of chemistry is now rapidly growing and he is the pioneer of this important area of chiral super Brønsted acid catalysis.

General Foundation of Acid Catalysis

Professor Yamamoto's contribution to organic chemistry is not limited to asymmetric synthesis. The above contribution to asymmetric acid catalysis was based on his pioneering study in Lewis acid reagents. He was intrigued by the chemistry of the carbonyl group-Lewis acid complex and introduced the unusually bulky organoaluminum reagents methylaluminum bis(2,6-di-tert-butyl-4-methylphenoxide) (MAD) and aluminum tris(2,6-diphenylphenoxide) (ATPH). These reagents were successfully utilized for the selective alkylation of cyclic ketones and aldehydes to generate equatorial alcohol and an *anti*-Cram-type product, respectively, for perfect *trans*- and *cis*-selective Claisen rearrangement, for regioselective and exo-selective Diels-Alder reaction, and for epoxide-aldehyde rearrangement. The ATPH-aromatic carbonyl complex selectively reacts with nucleophiles at the *para*-position of the aromatic ring to generate cyclohexadiene derivatives. Besides these unique and unexpected contributions to Lewis acid chemistry, his groundbreaking research in the area of organoaluminum chemistry has had a great impact on synthetic organic chemistry today. The strong Lewis acidity of organoaluminum compounds appears to account for their strong tendency to form a stable 1:1 complex. Thus, the coordination of Lewis acid to molecules invariably causes a change in reactivity and, though coordinated by Lewis acid, the group may be activated or deactivated depending upon the type of reaction. Furthermore, with the coordination of organic molecules, an auxiliary bond can become coupled to the reagent and promote the designed reaction. In short, the reagents make a combined Lewis acid-Lewis base attack on a substrate with less activation energy, a field opened by Yamamoto's early and highly original studies, which began in 1973. His aluminum amide reagents for epoxide rearrangement, biogenetic-type terpene synthesis, and the Beckmann rearrangement-alkylation reaction sequence are notable examples. Even more recently, Lewis acid-coordinated heterocyclic compounds are able to activate a specific position of the molecule for CH activation, which originated in Yamamoto’s Lewis acid chemistry: the work by Professor Nakao at Kyoto University. Based on these careful investigations of selective Lewis acid/Lewis base complexation, he proposed several basic principles for acetal chemistry, which are now used in the selective ring opening and alkylation processes for various asymmetric syntheses.

Finally, using this crucial information of Lewis and Brønsted acid catalysis, he recently achieved super silyl (tris(trimethylsilyl)silyl) chemistry, which can realize double or triple aldol reaction in a single pot to generate a number of stereogenic centers in the molecule. Otherwise unattainably high diastereoselectivity in this cascade reaction makes this process a so-called "second generation Mukaiyama aldol reaction", which can produce up to an eleven hydroxyl polyketide structure in three steps in a stereospecific manner. These findings open the possibility for a polyketide synthesizer, heretofore only dreamed of.

Designer Acid Catalysis

Yamamoto was intrigued by the chemistry of carbonyl group-Lewis acid complexes and introduced the unusually bulky organoaluminum reagents methylaluminum bis(2,6-di-tert-butyl-4-methylphenoxide) (MAD) and aluminum tris(2,6-diphenylphenoxide) (ATPH). These reagents were successfully utilized for the selective alkylation of cyclic ketones and aldehydes to generate equatorial alcohol and an *anti*-Cram-type product, respectively, for *trans*- and *cis*-selective Claisen rearrangement, for regioselective and exo-selective Diels-Alder reaction, and for epoxide-aldehyde rearrangement. The ATPH-aromatic carbonyl complex selectively reacts with nucleophiles at the *para*-position of the aromatic ring to generate cyclohexadiene derivatives. Besides these unexpected contributions to Lewis acid chemistry, his research in the area of organoaluminum chemistry has had a great impact on synthetic organic chemistry. The strong Lewis acidity of organoaluminum compounds appears to account for their strong tendency to form a stable 1:1 complex. Thus, the coordination of designer Lewis acid to molecules invariably causes a change in reactivity and, though coordinated by Lewis acid, the group may be activated or deactivated depending upon the type of reaction. Furthermore, with the coordination of organic molecules, an auxiliary bond can become coupled to the reagent and promote the designed reaction. In short, the reagents make a combined Lewis acid-Lewis base attack on a substrate with less activation energy, a field opened by Yamamoto's highly original early studies, which began in 1973. His aluminum amide reagents for epoxide rearrangement, biogenetic-type terpene synthesis, and the Beckmann rearrangement-alkylation reaction sequence are notable examples. Various Lewis acid-coordinated heterocyclic compounds are reported recently to activate specific positions of a molecule for CH activation, which originated in Yamamoto's Lewis acid chemistry. Based on these careful investigations of selective Lewis acid/Lewis base complexation, he proposed several basic principles for acetal chemistry, which are now used in selective ring opening and alkylation processes for various asymmetric syntheses. More recently, his ATPH catalyst is now used for the 1000-ton scale synthesis of perfumes in Japan.

Finally, using this crucial understanding of Lewis and Brønsted acid catalysis, he achieved super silyl (tris(trimethylsilyl)silyl) chemistry, which can realize double or triple aldol reactions in a single pot to generate a number of stereogenic centers in the molecule. Otherwise unattainably high diastereoselectivity in this cascade reaction makes this process a so-called "second generation of Mukaiyama aldol reaction", which can produce up to an eleven-hydroxyl polyketide structure only in three steps in a stereospecific manner. These findings open the new chapter for a polyketide synthesis in modern organic chemistry.

Other Catalytic Asymmetric Transformations

Professor Yamamoto also contributes significantly in the area of catalytic asymmetric oxidation reactions. For example, the nitroso-aldol reaction originated from his invention of O-nitroso aldol reaction over 10 years ago. Asymmetric epoxidation of homo- and bis-homoallylic alcohol was achieved first in his laboratory. His tungsten chemistry was a real groundbreaking discovery for oxidation using this non-toxic metal catalyst. Sequential epoxidation/ring opening will be used for a new strategy to generate >99.9%ee amino alcohol synthesis. The following is a list of catalytic asymmetric processes developed by Yamamoto: O-nitro aldol and N-nitroso aldol synthesis; nitroso-Diels-Alder reaction; epoxidations of homo- and bis-homoallylic alcohol; asymmetric S_N2 cross-coupling with carbonyl and allylic nucleophiles. Most of these reactions are classified by substrate-directed chemical reactions: Nonbonding interactions contributed by substrate substituents provide the dominant stereochemical control element for chemical transformations. In fact, his recent accomplishment of first catalytic peptide synthesis by Ta/Nb catalyst is a typical substrate directed chemical reaction.

Destructive Innovation for Peptide Synthesis

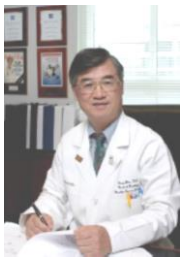
Direct condensation of carboxylic acids with alcohols or amines is the most important transformation of organic synthesis. His zirconium- or hafnium-catalyzed esterification and boron-catalyzed amidation were ground-breaking studies. More recently, Yamamoto discovered Lewis acid catalyzed peptide synthesis. With this information in hand, he discovered a new method for peptide synthesis using a tantalum Lewis acid catalyst. Efficient peptide synthesis has remained an unsolved problem in organic synthesis for over fifty years. Although Merrifield's solid phase peptide synthesis was a real breakthrough in 1963, unfortunately a real innovation has not appeared for more than 50 years! This classical method has three problems: unable to limit racemization; (2) linear synthesis and inability to devise a convergent process because of the lack of general ligation methodology; (3) requirement of protection/deprotection steps which requires a number of steps. His Lewis acid system finally solved all these three problems. His catalytic method provides synthesis of various peptides without any racemization by convergent synthesis, which proceeds in very few steps with much less expense (less than one thousandth to ten thousandth of the cost). Thus, Yamamoto's contribution finally provides a long-awaited opportunity for the drug industry desired since the last century. His Lewis acid peptide synthesis (LAPS) will facilitate an industrial synthetic approach for various peptide drugs in the coming years!

Yamamoto has published ~600 papers and numerous reviews and books, which have been cited more than >30,000 times (>50000 including books), with an h-index of 97 (113 by Google).

His contributions have been recognized by his being a recipient of, among others, the Prelog Medal (1993), the Chemical Society of Japan Award (1995), Le Grand Prix de la Fondation Maison de la Chimie (2002), the National Prize of Purple Medal (Japan) (2002), the Tetrahedron Prize for Creativity in Organic Chemistry (2006), the Japan Academy Award (2007), the Grand Prize of Synthetic Organic Chemistry of Japan (2009), the ACS Award for Creative Work in Synthetic Organic Chemistry (2009), Fellow of American Academy Arts and Science (2011), the Noyori Prize (2011), the Fujiwara Prize (2012), and the Roger Adams Award (2017) which is the highest award for organic chemistry in the US. The Person of Cultural Merit (2018), Barluenga Lectureship medal in Spain (2018), Member of EU Academy of Sciences (2019).

Phase II Trial of Paclitaxel, Ifosfamide & Cisplatin in Patients with Recurrent Head & Neck Squamous Cell Carcinoma

by Dong Moon Shin, Member EUAS



Short Biography

Dong Moon Shin, MD, FACP, FAAAS
Professor of Medical Oncology and Francis Kelly Blomeyer Chair in Cancer Research
Emory University School of Medicine

Dr. Dong Moon Shin is currently Professor of Medical Oncology, Otolaryngology and Biomedical Engineering, and holds Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research in the Department of Hematology and Medical Oncology at Winship Cancer Institute of Emory University. He graduated from Yonsei University College of Medicine and trained for Residency in Internal Medicine at Cook County Hospital, Chicago, IL and Medical Oncology at the University of Texas M. D. Anderson Cancer Center, Houston, TX. He has served as a faculty member in the Department of Thoracic/Head and Neck Medical Oncology at M. D. Anderson Cancer Center and University of Pittsburgh as Professor and Director of Head and Neck Cancer Program before he joined Emory University.

Honors and Awards

2018- Present Member of the EU Academy of Sciences (EUAS)
2017 Best Doctors in America (Oncology) (2003-2017)
2016 Top Doctors (Oncology) in Atlanta Magazine (Consecutively for 11 years)
2016 Member of the "Millipub" club (2,000 citations) of the Emory UniversitySchool of Medicine {NEJM 354: 567-78, 2006.}
2016 Elected Fellow of American Association of the Advancement of Science(FAAAS)
2015 Member of the "Millipub" club (2 articles cited more than 1000 times) of the Emory University School of Medicine {Nature Biotech. 26(1):83-90,
2008; Nature Rev. Drug Discovery. 7:771-82, 2008.}
2015 The 18th KBS (Korean Broadcasting System) Global Korean Award: Science and Technology
2014 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd. (Consecutively for 8 years)
2013/2012 Top Doctors featured in U.S. News & World Report
2011 Member of "Millipub" (article cited more than 1000 times) club of the Emory University School of Medicine {NEJM. 345:567-578, 2006.}
2010 Top Doctors (Oncology) in Atlanta Magazine
2010 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd.
2009 (Oct.) Honorary Professor at Central South University, Changsha, China
2009 Americas Top Doctors in Cancer by Castle Connolly Medical, Ltd
2009 Best Doctors in America (Oncology)
2009 Top Doctors (Oncology) in Atlanta Magazine
2009 Awardee of the Grand Prize for Medical Science in 2009 by Yonsei University, Seoul, Korea
2008 Top Doctors (Oncology) in Atlanta Magazine
2008 America's Top Doctors in Cancer by Castle Connolly Medical, Ltd.
2008 Frances Kelly Blomeyer Distinguished Endowed Chair in Cancer Research
2007 Cambridge Who's Who Life Time Member
2007 America's Top Oncologists by Consumers' Research Council of America

2005 Best Doctors in America (Oncology)
2005 Georgia Cancer Coalition (GCC) Distinguished Scholar Award
2005 Top Doctors (Oncology) in Atlanta
2004 Best Doctors in America
2003 Best Doctors in America
2001 Doris Duke Distinguished Clinical Scientist Award Nominee, Universityof Pittsburgh
2000 Faculty Scholar Award Nominee, M. D. Anderson Cancer Center
1994 Marquis Who's Who in the South and Southwest
1994 Distinguished Leadership Award for Cancer Research, American Biographical Institute, Inc.
1992 Fellowship of American College of Physicians
1994 Recipient of Clinical Oncology Career Development Award, American Cancer Society
1989 Who's Who in Medical Specialty
1987 Award of University Cancer Foundation (UCF) Research Funds

Phase II trial of paclitaxel, ifosfamide, and cisplatin in patients with recurrent head and neck squamous cell carcinoma

Citation

Shin DM, Glisson BS, Khuri FR, Ginsberg L, Papadimitrakopoulou V, Lee JJ, Lawhorn K, Gillenwater AM, Ang KK, Clayman GL, Callender DL, Hong WK, Lippman SM. Phase II trial of paclitaxel, ifosfamide, and cisplatin in patients with recurrent head and neck squamous cell carcinoma. J Clin Oncol. 1998 Apr;16(4):1325-30. doi: 10.1200/JCO.1998.16.4.1325. PMID: 9552033.

Abstract

Purpose: To assess the activity and toxicity profile of combined taxol (paclitaxel), ifosfamide, and platinum (cisplatin) (TIP) in patients with recurrent or metastatic squamous cell carcinoma (SCC) of the head and neck.
Patients and methods: Recurrent or metastatic head and neck SCC patients received paclitaxel 175 mg/m2 in a 3-hour infusion on day 1; ifosfamide 1,000 mg/m2 in a 2-hour infusion on days 1 through 3; mesna 600 mg/m2 on days 1 through 3; and cisplatin 60 mg/m2 on day 1, repeated every 3 to 4 weeks. All were premedicated with dexamethasone, diphenhydramine, and cimetidine. Prophylactic hematopoietic growth factors were not permitted.
Results: Fifty-two patients were assessable for response and toxicity; 53 for survival (local-regional recurrence alone in 57% and distant metastasis with or without local-regional recurrence in 43%). Overall response rate was 58% (30 of 52) of patients; complete response rate was 17% (nine of 52) of patients, with six complete responses that continued for a median 15.7+ months. Median follow-up of all patients was 17.7 months. Median survival was 8.8 months (95% confidence interval [CI] 8.1 to 17.5 months). Toxicity was relatively well tolerated and caused no deaths. The most frequent moderate-to-severe toxicity (90% of patients) was transient grades 3 to 4 neutropenia; neutropenic fever occurred in 27%. Grade 3 peripheral neuropathy occurred in three patients, none had grade 4. Grade 3 mucositis occurred in only one patient, none had grade 4.
Conclusion: TIP had major activity in this setting, with a 58% objective response rate, 17% complete response rate, durable complete responses (six of nine persisting), and relatively well-tolerated toxicity, with no toxic deaths. The activity of TIP, a novel taxol-cisplatin-based regimen, in recurrent or metastatic head and neck SCC should be confirmed in a phase III trial.

Combined interferon-alfa, 13-cis-retinoic acid, and alpha-tocopherol in locally advanced head and neck squamous cell carcinoma: novel bioadjuvant phase II trial

Citation

Shin DM, Khuri FR, Murphy B, Garden AS, Clayman G, Francisco M, Liu D, Glisson BS, Ginsberg L, Papadimitrakopoulou V, Myers J, Morrison W, Gillenwater A, Ang KK, Lippman SM, Goepfert H, Hong WK. Combined interferon-alfa, 13-cis-retinoic acid, and alpha-tocopherol in locally advanced head and neck squamous cell carcinoma: novel bioadjuvant phase II trial. J Clin Oncol. 2001 Jun 15;19(12):3010-7. doi: 10.1200/JCO.2001.19.12.3010. PMID: 11408495.

Abstract

Purpose: Retinoids and interferons (IFNs) have single-agent and synergistic combined effects in modulating cell proliferation, differentiation, and apoptosis in vitro and clinical activity in vivo in the head and neck and other sites. Alpha-tocopherol has chemopreventive activity in the head and neck and may decrease 13-cis-retinoic acid (13-cRA) toxicity. We designed the present phase II adjuvant trial to prevent recurrence or second primary tumors (SPTs) using 13-cRA, IFN-alpha, and alpha-tocopherol in locally advanced-stage head and neck cancer.

Patients and methods: After definitive local treatment with surgery, radiotherapy, or both, patients with locally advanced SCCHN were treated with 13-cRA (50 mg/m(2)/d, orally, daily), IFN-alpha (3 x 10(6) IU/m(2), subcutaneous injection, three times a week), and alpha-tocopherol (1,200 IU/d, orally, daily) for 12 months, with a dose modification. Screening for recurrence or SPTs was performed every 3 months.

Results: Tumors of 11 (24%) of the 45 treated patients were stage III, and 34 (76%) were stage IV. Thirty-eight (86%) of 44 patients completed the full 12-month treatment (doses modified as needed). Toxicity generally was consistent with previous IFN and 13-cRA reports and included mild to moderate mucocutaneous and flu-like symptoms; occasional significant fatigue (grade 3 in 7% of patients), mild to moderate hypertriglyceridemia in 30% of patients who continued treatment along with antilipid therapy, and mild hematologic side effects. Six patients did not complete the planned treatment because of intolerable toxicity or social problems. At a median 24-months of follow-up, our clinical end point rates were 9% for local/regional recurrence (four patients), 5% for local/regional recurrence and distant metastases (two patients), and 2% for SPT (one patient), which was acute promyelocytic leukemia (ie, not of the upper aerodigestive tract). Median 1- and 2-year rates of overall survival were 98% and 91%, respectively, and of disease-free survival were 91% and 84%, respectively.

Conclusion: The novel biologic agent combination of IFN-alpha, 13-cRA, and alpha-tocopherol was generally well tolerated and promising as adjuvant therapy for locally advanced squamous cell carcinoma of the head and neck. We are currently conducting a phase III randomized study of this combination (v no treatment) to confirm these phase II study results.

Radiotherapy plus cetuximab for squamous-cell carcinoma of the head and neck.

Citation

Bonner JA, Harari PM, Giralt J, Azarnia N, **Shin DM,** Cohen RB, Jones CU, Sur R, Raben D, Jassem J, Ove R, Kies MS, Baselga J, Youssoufian H, Amellal N, Rowinsky EK, Ang KK. Radiotherapy plus cetuximab for squamous-cell carcinoma of the head and neck. N Engl J Med. 2006 Feb 9;354(6):567-78. doi: 10.1056/NEJMoa053422. PMID: 16467544.

Abstract

Background: We conducted a multinational, randomized study to compare radiotherapy alone with radiotherapy plus cetuximab, a monoclonal antibody against the epidermal growth factor receptor, in the treatment of locoregionally advanced squamous-cell carcinoma of the head and neck.

Methods: Patients with locoregionally advanced head and neck cancer were randomly assigned to treatment with high-dose radiotherapy alone (213 patients) or high-dose radiotherapy plus weekly cetuximab (211 patients) at an initial dose of 400 mg per square meter of body-surface area, followed by 250 mg per square meter weekly for the duration of radiotherapy. The primary end point was the duration of control of locoregional disease; secondary end points were overall survival, progression-free survival, the response rate, and safety.

Results: The median duration of locoregional control was 24.4 months among patients treated with cetuximab plus radiotherapy and 14.9 months among those given radiotherapy alone (hazard ratio for locoregional progression or death, 0.68; P=0.005). With a median follow-up of 54.0 months, the median duration of overall survival was 49.0 months among patients treated with combined therapy and 29.3 months among those treated with radiotherapy alone (hazard ratio for death, 0.74; P=0.03). Radiotherapy plus cetuximab significantly prolonged progression-free survival (hazard ratio for disease progression or death, 0.70; P=0.006). With the exception of acneiform rash and infusion reactions, the incidence of grade 3 or greater toxic effects, including mucositis, did not differ significantly between the two groups.

Conclusions: Treatment of locoregionally advanced head and neck cancer with concomitant high-dose radiotherapy plus cetuximab improves locoregional control and reduces mortality without increasing the common toxic effects associated with radiotherapy to the head and neck. (ClinicalTrials.gov number, NCT00004227.)

Nanoparticle therapeutics: an emerging treatment modality for cancer.

Citation

Davis ME, Chen ZG, **Shin DM.** Nanoparticle therapeutics: an emerging treatment modality for cancer. Nat Rev Drug Discov. 2008 Sep;7(9):771-82. doi: 10.1038/nrd2614. PMID: 18758474.

Abstract

Nanoparticles--particles in the size range 1-100 nm--are emerging as a class of therapeutics for cancer. Early clinical results suggest that nanoparticle therapeutics can show enhanced efficacy, while simultaneously reducing side effects, owing to properties such as more targeted localization in tumours and active cellular uptake. Here, we highlight the features of nanoparticle therapeutics that distinguish them from previous anticancer therapies, and describe how these features provide the potential for therapeutic effects that are not achievable with other modalities. While large numbers of preclinical studies have been published, the emphasis here is placed on preclinical and clinical studies that are likely to affect clinical investigations and their implications for advancing the treatment of patients

with cancer.

Chemoprevention of head and neck cancer by simultaneous blocking of epidermal growth factor receptor and cyclooxygenase-2 signaling pathways: preclinical and clinical studies.

Citation

Shin DM, Zhang H, Saba NF, Chen AY, Nannapaneni S, Amin AR, Müller S, Lewis M, Sica G, Kono S, Brandes JC, Grist WJ, Moreno-Williams R, Beitler JJ, Thomas SM, Chen Z, Shin HJ, Grandis JR, Khuri FR, Chen ZG. Chemoprevention of head and neck cancer by simultaneous blocking of epidermal growth factor receptor and cyclooxygenase-2 signaling pathways: preclinical and clinical studies. Clin Cancer Res. 2013 Mar 1;19(5):1244-56. doi: 10.1158/1078-0432.CCR-12-3149. Epub 2013 Feb 19. PMID: 23422093; PMCID: PMC3693760.

Abstract

Purpose: We investigated the efficacy and underlying molecular mechanism of a novel chemopreventive strategy combining EGF receptor (EGFR) tyrosine kinase inhibitor (TKI) with cyclooxygenase-2 inhibitor (COX-2I).

Experimental design: We examined the inhibition of tumor cell growth by combined EGFR-TKI (erlotinib) and COX-2I (celecoxib) treatment using head and neck cancer cell lines and a preventive xenograft model. We studied the antiangiogenic activity of these agents and examined the affected signaling pathways by immunoblotting analysis in tumor cell lysates and immunohistochemistry (IHC) and enzyme immunoassay (EIA) analyses on the mouse xenograft tissues and blood, respectively. Biomarkers in these signaling pathways were studied by IHC, EIA, and an antibody array analysis in samples collected from participants in a phase I chemoprevention trial of erlotinib and celecoxib.

Results: The combined treatment inhibited head and neck cancer cell growth significantly more potently than either single agent alone in cell line and xenograft models, and resulted in greater inhibition of cell-cycle progression at G1 phase than either single drug. The combined treatment modulated the EGFR and mTOR signaling pathways. A phase I chemoprevention trial of combined erlotinib and celecoxib revealed an overall pathologic response rate of 71% at time of data analysis. Analysis of tissue samples from participants consistently showed downregulation of EGFR, pERK, and pS6 levels after treatment, which correlated with clinical response.

Conclusion: Treatment with erlotinib combined with celecoxib offers an effective chemopreventive approach through inhibition of EGFR and mTOR pathways, which may serve as potential biomarkers to monitor the intervention of this combination in the clinic. Clin Cancer Res; 19(5); 1244-56. ©2013 AACR.

Phase Ib Study of Chemoprevention with Green Tea Polyphenon E and Erlotinib in Patients with Advanced Premalignant Lesions (APL) of the Head and Neck

Citation

Shin DM, Nannapaneni S, Patel MR, Shi Q, Liu Y, Chen Z, Chen AY, El-Deiry MW, Beitler JJ, Steuer CE, Roser SM, Klein AM, Owonikoko TK, Ramalingam SS, Khuri FR, Chen ZG, Saba NF. Phase Ib Study of Chemoprevention with Green Tea Polyphenon E and Erlotinib in Patients with Advanced Premalignant Lesions (APL) of the Head and

Neck. Clin Cancer Res. 2020 Nov 15;26(22):5860-5868. doi: 10.1158/1078-0432.CCR-20-2276. Epub 2020 Sep 17. PMID: 32943457.

Abstract

Purpose: On the basis of synergistic effects between green tea polyphenon E (PPE) and EGFR-tyrosine kinase inhibitor in preclinical studies, we conducted a phase Ib study of the PPE and erlotinib combination in patients with advanced premalignant lesions (APL) of the oral cavity and larynx.

Patients and methods: Patients were treated with a fixed dose of PPE (200 mg three times a day) and dose escalation of erlotinib (50, 75, 100 mg daily) for 6 months with tissue biopsy at baseline and 6 months. Primary endpoints were safety and toxicity; secondary endpoints were evaluation of pathologic response, cancer-free survival (CFS), overall survival (OS), and biomarker modulation.

Results: Among 21 enrolled patients, 19 began treatment and 17 completed 6 months of treatment with PPE and erlotinib. Main characteristics of treated patients: 15 severe dysplasia or carcinoma in situ and 17 oral cavity. Only skin rash was associated with dose-limiting toxicity and MTD. Recommended doses for phase II studies are PPE 600 mg daily plus erlotinib 100 mg daily for 6 months. Pathologic responses in 17 evaluable patients: pathologic complete response (47%) and pathologic partial response (18%).

The 5-year CFS and OS were 66.3% and 93%, respectively. Among tested biomarkers, only phosphorylated ERK was correlated with response to treatment.

Conclusions: Treatment with PPE and erlotinib combination was well tolerated in patients with APLs of the head and neck, and showed a high rate of pathologic response with excellent CFS. This combination deserves further investigation for the chemoprevention and/or prevention of second primary tumors in early-stage head and neck cancer.

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Dreaming of No More Renal Dialysis Kidney Graft Survival in Rats without Immunosuppressants after Intrathymic Glomerular Transplantation

by Giuseppe Remuzzi, Member EUAS

Short Biography

Giuseppe Remuzzi completed his medical training at the University of Pavia in 1974 and then received specialty training in Haematology and Nephrology at the University of Milan in 1977 and 1980, respectively. From 1996 until 2013 he was Director of the public-private Department of Immunology and Transplant Medicine (a collaboration between the Ospedali Riuniti of Bergamo and the Mario Negri Institute) and from 1999 until 2018 he has also been Head of the Division of Nephrology and Dialysis. From 2011 until 2015 he was Director of the Department of Medicine of the Azienda Ospedaliera Papa Giovanni XXIII (formerly the Ospedali Riuniti) of Bergamo. In June 2015 he was nominated Chiara Fama Professor of Nephrology at the University of Milan. Alongside his clinical work in hospital, Prof. Remuzzi has dedicated himself to intense didactic and research activities. Since the Mario Negri Institute for Pharmacological Research opened its branch in Bergamo, Prof. Remuzzi has coordinated all of the research that takes place there, and since 1992 he has done the same for the Aldo e Cele Daccò Clinical Research Centre for Rare Diseases in Ranica, Bergamo. Since July 1st Professor Remuzzi has also taken on the role of Director of the the Mario Negri Institute. His main research interests include the causes of glomerulonephritis and the mechanisms of progression of kidney diseases. He has also conducted many studies in the field of transplant rejection. With an innovative approach (transplanting two kidneys from older donors into one recipient, after carefully evaluating the condition of the organs), his research has facilitated an increase in the number of transplants conducted. His most recent research concerns the possibility of regenerating tissues and creating organs in the laboratory using stem cells.

Prof. Remuzzi serves on editorial boards of numerous journals and is member of the International Advisory Board of The Lancet. He served as Editorial Board member of the New England Journal of Medicine from 1998-2013. In recognition of his achievements, he has been awarded in 1998 honorary memberships of the Association of American Physicians and the British Royal College of Physicians. In 2005 during the World Congress of Nephrology in Singapore he received the ISN Jean Hamburger Award. In 2007 he received during the annual American Society of Nephrology Congress in San Francisco the prestigious ASN John P. Peters Award and in 2011 he was awarded with the ISN AMGEN Award (World Congress of Nephrology: WCN 2011, Vancouver). In November 2011 he received the Third Edition of the International Award "Luis Hernando" assigned by the Iñigo Alvarez de Toledo Renal Foundation (FRIAT) in Madrid, Spain.

From June 2013 until March 2015 he was President of the International Society of Nephrology (ISN). During his tenure he created and launched the global 0by25 project, the goal of which is that "Nobody should die of preventable and treatable Acute Kidney Injury (AKI) by 2025".

In April 2018 he was awaded the "Lennox K. Black International Prize for Excellence in Medicine" at the Thomas Jefferson University in Philadelphia.

Prof. Remuzzi is the author of over 1450 publications in International medical journals and has written 16 books. He also regularly writes editorials for the Corriere della Sera newspaper.

Kidney graft survival in rats without immunosuppressants after intrathymic glomerular transplantation

G.Remuzzi, M.Rossini O.Imberti N.Perico
Lancet 1991; 337:750-752

Abstract
Isolated glomeruli from Brown-Norway (RT1n) rat kidney were inoculated into the thymus of 6 incompatible Lewis (RT11) rats pretreated for 2 days with 40 mg/kg oral cyclosporin daily and given 2·5 mg/kg subcutaneous dexamethasone at inoculation. 10 days later the left kidney from the Brown-Norway donor used to prepare glomeruli was transplanted orthotopically to the Lewis (RT11) rat that had received intrathymic glomeruli. Donor-specific unresponsiveness allowed the renal allograft to survive indefinitely without further immunosuppression. 6 control Lewis rats treated as above except that medium alone was injected intrathymically rejected a renal allograft within 7-9 days.

Randomised placebo-controlled trial of effect of ramipril on decline in glomerular filtration rate and risk of terminal renal failure in proteinuric, non-diabetic nephropathy

The GISEN Group (Gruppo Italiano di Studi Epidemiologici in Nefrologia)
The Lancet Volume 349, Issue 9069, 28 June 1997, Pages 1857-1863

Summary
Background
In diabetic nephropathy, angiotensin-converting-enzyme (ACE) inhibitors have a greater effect than other antihypertensive drugs on proteinuria and the progressive decline in glomerular filtration rate (GFR). Whether this difference applies to progression of non-diabetic proteinuric nephropathies is not clear. The Ramipril Efficacy In Nephropathy study of chronic non-diabetic nephropathies aimed to address whether glomerular protein traffic influences renal-disease progression, and whether an ACE inhibitor was superior to conventional treatment, with the same blood-pressure control, in reducing proteinuria, limiting GFR decline, and preventing endstage renal disease.
Methods
In this prospective double-blind trial, 352 patients were classified according to baseline proteinuria (stratum 1: 1–3 g/24 h; stratum 2: ≥3 g/24 h), and randomly assigned ramipril or placebo plus conventional antihypertensive therapy targeted at achieving diastolic blood pressure under 90 mm Hg. The primary endpoint was the rate of GFR decline. Analysis was by intention to treat.
Finding
At the second planned interim analysis, the difference in decline in GFR between the ramipril and placebo groups in stratum 2 was highly significant (p=0·001). The Independent Adjudicating Panel therefore decided to open the randomisation code and do the final analysis in this stratum (stratum 1 continued in the trial). Data (at least three GFR measurements including baseline) were available for 56 ramipril-assigned patients and 61 placebo-assigned patients. The decline in GFR per month was significantly lower in the ramipril group than the placebo group (0·53 [0·08] vs 0·88 [0·13] mL/min, p=0·03). Among the ramipril-assigned patients, percentage reduction in proteinuria was inversely correlated with decline in GFR (p=0·035) and predicted the reduction in risk of doubling of baseline creatinine or endstage renal failure (18 ramipril vs 40 placebo, p=0·04). The risk of progression was still significantly reduced after adjustment for changes in systolic (p=0·04) and diastolic (p=0·04) blood pressure, but not after adjustment for changes in

proteinuria. Blood-pressure control and the overall number of cardiovascular events were similar in the two treatment groups.
Interpretation
In chronic nephropathies with proteinuria of 3 g or more per 24 h, ramipril safely reduces proteinuria and the rate of GFR decline to an extent that seems to exceed the reduction expected for the degree of blood-pressure lowering.

Pathophysiology of Progressive Nephropathies

Giuseppe Remuzzi, M.D., and Tullio Bertani, M.D.
N Engl J Med 1998; 339:1448-1456

In patients with renal diseases characterized by proteinuria, the initial insult to the kidney is usually followed by a progressive decline in the glomerular filtration rate. This decline has been thought to be due to changes in renal hemodynamics initiated by the loss of nephrons.1 When renal mass is reduced in rats, the remaining nephrons undergo sudden hypertrophy, with a concomitant lowering of arteriolar resistance and an increase in glomerular plasma flow.2,3 Afferent arteriolar tone decreases more than efferent arteriolar tone, and therefore, the hydraulic pressure in glomerular capillaries rises4 and the amount of filtrate formed by each nephron increases. These changes increase the filtration capacity of the remaining nephrons, thus minimizing the functional consequences of nephron loss, but they are ultimately detrimental.5 Therapies that attenuate these adaptive changes limit the decline in the glomerular filtration rate and minimize structural damage. For example, angiotensin-converting–enzyme (ACE) inhibitors, which reduce intraglomerular capillary pressure more effectively than other antihypertensive drugs, consistently protected rats with reduced renal mass6,7 or diabetes mellitus8,9 from progressive renal injury.

Why should hemodynamic changes — specifically, glomerular hypertension — lead to progressive renal injury? One possible explanation is that the high glomerular capillary pressure enlarges the radius of the pores in the glomerular membrane by a mechanism that is mediated at least in part by angiotensin II.10,11 This enlargement impairs the size-selective function of the membrane so that the protein content of the glomerular filtrate increases, which in turn increases the endocytosis of protein by tubular epithelial cells, ultimately resulting in a nephritogenic effect.12 A vicious circle is then established in which changes in renal hemodynamics due to the loss of nephrons lead first to proteinuria and then to the loss of more nephrons.

Effect of Increased Glomerular Permeability to Proteins on Progressive Renal Injury.
We will review recent data suggesting that proteins filtered by the glomerulus cause injury of the tubulointerstitium, leading to parenchymal damage and, ultimately, renal scarring and insufficiency (Figure 1). We will also review experimental and clinical evidence linking the renoprotective effects of ACE inhibitors to their ability to reduce the levels of protein in the glomerular filtrate, as well as the predictive value of the degree of proteinuria in determining the rate of progression of chronic renal diseases characterized by abnormal loss of proteins into the urine — that is, proteinuric nephropathies.

Rituximab for idiopathic membranous nephropathy

Lancet 2002 Sep 21;360(9337):923-4.

Giuseppe Remuzzi 1 , Carlos Chiurchiu, Mauro Abbate, Verusca Brusegan, Mario Bontempelli, Piero Ruggenenti

Abstract
Treatments for idiopathic membranous nephropathy, a common cause of nephrotic syndrome, can be very toxic. In view of the pathogenic potential of B cells in this disease, we studied the effects of four weekly infusions of rituximab (375 mg/m(2)-- the monoclonal antibody to B-cell antigen CD20--in eight patients who had idiopathic membranous nephropathy with persistent nephrotic syndrome. At weeks 4 and 20, urinary protein decreased from mean (SE) 8.6 g/24 h (1.4) to 3.8 (0.8) and 3.7 (0.9), respectively ($p<0.0001$). At week 20, albuminuria and albumin fractional clearance decreased by 70% and 65%, and serum albumin increased by 31%. CD20 B lymphocytes fell below normal ranges up to study end. The short-term risk-benefit profile of rituximab seems more favourable to that of any other immunosuppressive drug used to treat idiopathic membranous nephropathy.

Preventing Microalbuminuria in Type 2 Diabetes

Piero Ruggenenti, M.D., Anna Fassi, M.D., Anelja Parvanova Ilieva, M.D., Simona Bruno, M.D., Ilian Petrov Iliev, M.D., Varusca Brusegan, M.D., Nadia Rubis, R.N., Giulia Gherardi, R.N., Federica Arnoldi, R.N., Maria Ganeva, Stat.Sci.D., Bogdan Ene-Iordache, Eng.D., Flavio Gaspari, Ph.D., et al., for the Bergamo Nephrologic Diabetes Complications Trial (BENEDICT) Investigators
N Engl J Med 2004; 351:1941-1951

The multicenter double-blind, randomized Bergamo Nephrologic Diabetes Complications Trial (BENEDICT) was designed to assess whether angiotensin-converting–enzyme inhibitors and non-dihydropyridine calcium-channel blockers, alone or in combination, prevent microalbuminuria in subjects with hypertension, type 2 diabetes mellitus, and normal urinary albumin excretion.

Methods
We studied 1204 subjects, who were randomly assigned to receive at least three years of treatment with trandolapril (at a dose of 2 mg per day) plus verapamil (sustained-release formulation, 180 mg per day), trandolapril alone (2 mg per day), verapamil alone (sustained-release formulation, 240 mg per day), or placebo. The target blood pressure was 120/80 mm Hg. The primary end point was the development of persistent microalbuminuria (overnight albumin excretion, ≥20 μg per minute at two consecutive visits).

Results
The primary outcome was reached in 5.7 percent of the subjects receiving trandolapril plus verapamil, 6.0 percent of the subjects receiving trandolapril, 11.9 percent of the subjects receiving verapamil, and 10.0 percent of control subjects receiving placebo. The estimated acceleration factor (which quantifies the effect of one treatment relative to another in accelerating or slowing disease progression) adjusted for predefined baseline characteristics was 0.39 for the comparison between verapamil plus trandolapril and placebo (P=0.01), 0.47 for the comparison between trandolapril and placebo (P=0.01), and 0.83 for the comparison between verapamil and placebo (P=0.54). Trandolapril plus verapamil and trandolapril alone delayed the onset of microalbuminuria by factors of 2.6

and 2.1, respectively. Serious adverse events were similar in all treatment groups.

Conclusions
In subjects with type 2 diabetes and hypertension but with normoalbuminuria, the use of trandolapril plus verapamil and trandolapril alone decreased the incidence of microalbuminuria to a similar extent. The effect of verapamil alone was similar to that of placebo.

Long-Term Outcome of Renal Transplantation from Older Donors

Giuseppe Remuzzi, M.D., Paolo Cravedi, M.D., Annalisa Perna, Stat.Sci.D., Borislav D. Dimitrov, M.D., M.Sc., Marta Turturro, Biol.Sci.D., Giuseppe Locatelli, M.D., Paolo Rigotti, M.D., Nicola Baldan, M.D., Marco Beatini, M.D., Umberto Valente, M.D., Mario Scalamogna, M.D., and Piero Ruggenenti, M.D. for the Dual Kidney Transplant Group*
N Engl J Med 2006; 354:343-352

Abstract
Background
Long-term survival of kidney grafts from older donors is inferior to that of grafts from younger donors. We sought to determine whether selecting older kidneys according to their histologic characteristics before implantation would positively influence long-term outcome.
Methods
In a prospective cohort study, we assessed outcomes among 62 patients who received one or two histologically evaluated kidneys from donors older than 60 years of age. These outcomes were compared with outcomes among 248 matched recipients of single kidney grafts that had not been histologically evaluated and were either from donors 60 years of age or younger (124 positive-reference recipients who, according to available data, were expected to have an optimal outcome) or from those older than 60 years (124 negative-reference recipients, expected to have a worse outcome). The primary end point was graft survival.
Results
During a median period of 23 months, 4 recipients (6 percent) of histologically evaluated kidneys progressed to dialysis, as compared with 7 positive-reference recipients (6 percent) and 29 negative-reference recipients (23 percent). Graft survival in recipients of histologically evaluated kidneys did not differ significantly from that of grafts in positive-reference recipients but was superior to that of grafts in negative-reference recipients (hazard ratio for graft failure in the negative-reference recipients relative to the recipients of histologically evaluated kidneys, 3.68; 95 percent confidence interval, 1.29 to 10.52; P=0.02). The performance of preimplantation histologic evaluation predicted better survival both in the whole study group (P=0.02) and among recipients of kidneys from older donors (P=0.01).
Conclusions
The long-term survival of single or dual kidney grafts from donors older than 60 years of age is excellent, provided that the grafts are evaluated histologically before implantation. This approach may help to expand the donor-organ pool for kidney transplantation.

MYO1E Mutations and Childhood Familial Focal Segmental Glomerulosclerosis

Caterina Mele, Biol.Sci.D., Paraskevas Iatropoulos, M.D., Roberta Donadelli, Biol.Sci.D., Andrea Calabria, Eng.D., Ramona Maranta, Biol.Sci.D., Paola Cassis, Ph.D., Simona Buelli, Ph.D., Susanna Tomasoni, Ph.D., Rossella Piras, Chem.Pharm.D., Mira Krendel, Ph.D., Serena Bettoni, Biotech.D., Marina Morigi, Ph.D., Massimo Delledonne, Ph.D., Carmine Pecoraro, M.D., Isabella Abbate, Ph.D., Maria Rosaria Capobianchi, Ph.D., Friedhelm Hildebrandt, M.D., Edgar Otto, M.D., Franz Schaefer, M.D., Fabio Macciardi, M.D., Fatih Ozaltin, M.D., Sevinc Emre, M.D., Tulin Ibsirlioglu, Ph.D., Ariela Benigni, Ph.D., Giuseppe Remuzzi, M.D., and Marina Noris, Ph.D. for the PodoNet
N Engl J Med 2011; 365:295-306

Abstract

Background

Focal segmental glomerulosclerosis is a kidney disease that is manifested as the nephrotic syndrome. It is often resistant to glucocorticoid therapy and progresses to end-stage renal disease in 50 to 70% of patients. Genetic studies have shown that familial focal segmental glomerulosclerosis is a disease of the podocytes, which are major components of the glomerular filtration barrier. However, the molecular cause in over half the cases of primary focal segmental glomerulosclerosis is unknown, and effective treatments have been elusive.

Methods

We performed whole-genome linkage analysis followed by high-throughput sequencing of the positive-linkage area in a family with autosomal recessive focal segmental glomerulosclerosis (index family) and sequenced a newly discovered gene in 52 unrelated patients with focal segmental glomerulosclerosis. Immunohistochemical studies were performed on human kidney-biopsy specimens and cultured podocytes. Expression studies in vitro were performed to characterize the functional consequences of the mutations identified.

Results

We identified two mutations (A159P and Y695X) in MYO1E, which encodes a nonmuscle class I myosin, myosin 1E (Myo1E). The mutations in MYO1E segregated with focal segmental glomerulosclerosis in two independent pedigrees (the index family and Family 2). Patients were homozygous for the mutations and did not have a response to glucocorticoid therapy. Electron microscopy showed thickening and disorganization of the glomerular basement membrane. Normal expression of Myo1E was documented in control human kidney-biopsy specimens in vivo and in glomerular podocytes in vitro. Transfection studies revealed abnormal subcellular localization and function of the A159P-Myo1E mutant. The Y695X mutation causes loss of calmodulin binding and of the tail domains of Myo1E.

Conclusions

MYO1E mutations are associated with childhood-onset, glucocorticoid-resistant focal segmental glomerulosclerosis. Our data provide evidence of a role of Myo1E in podocyte function and the consequent integrity of the glomerular filtration barrier.

Mesenchymal stromal cells in renal transplantation: opportunities and challenges

Casiraghi, Federica; Perico, Norberto; Cortinovis, Monica; Remuzzi, Giuseppe.
Nature Reviews. Nephrology; London Vol. 12, Iss. 4, (Apr 2016): 241-253. DOI:10.1038/nrneph.2016.7

Abstract
Lifelong immunosuppressive therapy is essential to prevent allograft rejection in transplant recipients. Long-term, nonspecific immunosuppression can, however, result in life-threatening complications and fail to prevent chronic graft rejection. Bone marrow (BM)-derived multipotent mesenchymal stromal cells (MSCs) have emerged as a potential candidate for cell-based therapy to modulate the immune response in organ transplantation. These cells can repair tissue after injury and downregulate many of the effector functions of immune cells that participate in the alloimmune response, converting them into regulatory cells. The findings of preclinical and initial clinical studies support the potential tolerance-inducing effects of MSCs and highlight the unanticipated complexity of MSC therapy in kidney transplantation. In animal models of transplantation MSCs promote donor-specific tolerance through the generation of regulatory T cells and antigen-presenting cells. In some settings, however, MSCs can acquire proinflammatory properties and contribute to allograft dysfunction. The available data from small clinical studies suggest that cell infusion is safe and well tolerated by kidney transplant recipients. Ongoing and future trials will provide evidence regarding the long-term safety of MSC therapy and determine the optimum cell source (either autologous or allogeneic) and infusion protocol to achieve operational tolerance in kidney transplant recipients. These studies will also provide additional evidence regarding the risks and benefits of MSC infusion and will hopefully offer definitive answers to the important questions of when, where, how many and which types of MSCs should be infused to fully exploit their immunomodulatory, pro-tolerogenic and tissue-repairing properties.

Experimental Evaluation of Kidney Regeneration by Organ Scaffold Recellularization

Andrea Remuzzi, Marina Figliuzzi, Barbara Bonandrini, Sara Silvani, Nadia Azzollini, Roberta Nossa, Ariela Benigni & Giuseppe Remuzzi
Scientific Reports volume 7, Article number: 43502 (2017) Cite this article

Abstract
The rising number of patients needing renal replacement therapy, alongside the significant clinical and economic limitations of current therapies, creates an imperative need for new strategies to treat kidney diseases. Kidney bioengineering through the production of acellular scaffolds and recellularization with stem cells is one potential strategy. While protocols for obtaining organ scaffolds have been developed successfully, scaffold recellularization is more challenging. We evaluated the potential of in vivo and in vitro kidney scaffold recellularization procedures. Our results show that acellular scaffolds implanted in rats cannot be repopulated with host cells, and in vitro recellularization is necessary. However, we obtained very limited and inconsistent cell seeding when using different infusion protocols, regardless of injection site. We also obtained experimental and theoretical data indicating that uniform cell delivery into the kidney scaffolds cannot be obtained using these infusion protocols, due to the permeability of the extracellular matrix of the scaffold. Our results highlight the major physical barriers that limit in vitro recellularization of acellular kidney scaffolds and the obstacles that must be investigated to effectively advance this strategy for regenerative medicine.

Mechanochemistry for Ammonia Synthesis under Mild Conditions

by Qing Jiang, Member EUAS

Short Biography

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

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

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

Dr. Jiang was elected as a Member of the EU Academy of Sciences in 2018, and an Academician of the Asia Pacific Academy of Materials in 2015. He is a Fellow of The Institute of Physics (U.K.), and several editor board members of academic journals.

Dr. Jiang current research interests include synthesis of nanomaterials as well as their applications in catalysis, energy storage and conversion (fuel cell, batteries, supercapacitors and electrocatalysis), emphasizing kinetics aspects of mass transfer and chemical reaction. He has published more than 600 papers in peer-reviewed journals, including Nat. Nanotechnol., Nat. Chem., Nat. Commun., Sci. Adv., Joule, Chem, Matter, et al. His publications have been cited more than 21,000 times with H-index = 74 (Web of Science).

In 2020, he authored and coauthored 52 papers and several with abstracts among them

are listed below:

1. G. F. Han, F. Li, Z. W. Chen, C. Coppex, S. J. Kim, H. J. Noh, Z. Fu, Y. Lu, C. V. Singh, S. Siahrostami , Q. Jiang, J. B. Baek, "Mechanochemistry for ammonia synthesis under mild conditions", Nat. Nanotechnol., 2020, https://doi.org/10.1038/s41565-020-00809-9

Abstract

Ammonia, one of the most important synthetic feedstocks, is mainly produced by the Haber-Bosch process at 400-500 °C and above 100 bar. The process cannot be performed under ambient conditions for kinetic reasons. Here, we demonstrate that ammonia can be synthesized at 45 °C and 1 bar via a mechanochemical method using an iron-based catalyst. With this process the ammonia final concentration reached 82.5 vol%, which is higher than state-of-the-art ammonia synthesis under high temperature and pressure (25 vol%, 450 °C, 200 bar). The mechanochemically induced high defect density and violent impact on the iron catalyst were responsible for the mild synthesis conditions.

2. H. Shi, Y. T. Zhou, R. Q. Yao, W. B. Wan, X. Ge, W. Zhang, Z. Wen, X. Y. Lang, W. T. Zheng, Q. Jiang, "Spontaneously separated intermetallic Co3Mo from nanoporous copper as versatile electrocatalysts for highly efficient water splitting", Nat. Commun. 2020, 11, 2940.

Abstract

Developing robust nonprecious electrocatalysts towards hydrogen/oxygen evolution reactions is crucial for widespread use of electrochemical water splitting in hydrogen production. Here, we report that intermetallic Co3Mo spontaneously separated from hierarchical nanoporous copper skeleton shows genuine potential as highly efficient electrocatalysts for alkaline hydrogen/oxygen evolution reactions in virtue of in-situ hydroxylation and electrooxidation, respectively. The hydroxylated intermetallic Co3Mo has an optimal hydrogenbinding energy to facilitate adsorption/desorption of hydrogen intermediates for hydrogen molecules. Associated with high electron/ion transport of bicontinuous nanoporous skeleton, nanoporous copper supported Co3Mo electrodes exhibit impressive hydrogen evolution reaction catalysis, with negligible onset overpotential and low Tafel slope (~40 mV dec−1) in 1 M KOH, realizing current density of −400 mA cm−2 at overpotential of as low as 96 mV. When coupled to its electro-oxidized derivative that mediates efficiently oxygen evolution reaction, their alkaline electrolyzer operates with a superior overall water-splitting output, outperforming the one assembled with noble-metal-based catalysts.

3. S. B. Wang, Q. Ran, R. Q. Yao, H. Shi, Z. Wen, M. Zhao, X. Y. Lang, Q. Jiang, "Lamella-nanostructured eutectic zinc-aluminum alloys as reversible and dendrite-free anodes for aqueous rechargeable batteries", Nat. Commun. 2020, 11, 1634.

Abstract

Metallic zinc is an attractive anode material for aqueous rechargeable batteries because of its high theoretical capacity and low cost. However, state-of-the-art zinc anodes suffer from low coulombic efficiency and severe dendrite growth during stripping/plating processes, hampering their practical applications. Here we show that eutectic-composition alloying of zinc and aluminum as an effective strategy substantially tackles these irreversibility issues by making use of their lamellar structure, composed of alternating zinc and aluminum nanolamellas. The lamellar nanostructure not only promotes zinc stripping from precursor eutectic Zn88Al12 (at%) alloys, but produces core/shell aluminum/aluminum sesquioxide interlamellar nanopatterns in situ to in turn guide subsequent growth of zinc, enabling dendritefree zinc stripping/plating for more than 2000 h in oxygen-absent aqueous electrolyte. These outstanding electrochemical properties enlist zinc-ion batteries constructed with Zn88Al12 alloy anode and KxMnO2 cathode to deliver high-density energy at high levels of electrical power and retain 100% capacity after 200 hours.

4. R. Q. Yao, H. Shi, W. B. Wan, Z. Wen, X. Y. Lang, Q. Jiang, "Flexible Co–Mo–N/Au Electrodes with a Hierarchical Nanoporous Architecture as Highly Effcient Electrocatalysts for Oxygen Evolution Reaction ", Adv. Mater. 2020, 32, 1907214.

Abstract

Designing highly active and robust electrocatalysts for oxygen evolution reaction (OER) is crucial for many renewable energy storage and conversion devices. Here, self-supported monolithic hybrid electrodes that are composed of bimetallic cobalt–molybdenum nitride nanosheets vertically aligned on 3D and bicontinuous nanoporous gold (NP Au/CoMoNx) are reported as highly effcient electrocatalysts to boost the sluggish reaction kinetics of water oxidation in alkaline media. By virtue of the constituent CoMoNx nanosheets having large accessible CoMoOx surface with remarkably enhanced electrocatalytic activity and the nanoporous Au skeleton facilitating electron transfer and mass transport, the NP Au/CoMoNx electrode exhibits superior OER electrocatalysis in 1 M KOH, with low onset overpotential (166 mV) and Tafel slope (46 mV dec-1). It only takes a low overpotential of 370 mV to reach ultrahigh current density of 1156 mA cm−2, ≈ 140-fold higher than free CoMoNx nanosheets. The electrocatalytic performance makes it an attractive candidate as the OER catalyst in the water electrolysis.

5. J. Han, A. Zhang, M. Chen, W. Gao, Q. Jiang, "Giant Rashba splitting in one-dimensional atomic tellurium chains", Nanoscale, 2020, 12, 10277

Abstract

The search for a one-dimensional (1D) system with purely 1D bands and strong Rashba spin splitting is essential for the realization of Majorana fermions and spin transport but presents a fundamental challenge to date. Herein, using first-principles calculations, we demonstrated that atomic Tellurium (Te) chains exhibit purely 1D bands and giant Rashba spin splitting, and their splitting parameters depend strongly on strain and structure distortion. This phenomenon stems from the helical structure of atomic Te chains, which can not only sustain significant strain but also realize the synergy of orbital angular momentum and in-chain potential gradient in enhancing spin splitting. The structure distortion of stretched helical Te chains is critical to execute this synergy, generating a large Rashba spin splitting among the known systems. Our findings proposed a potential 1D giant Rashba splitting system for exploring spintronics and Majorana fermions, and provide routes for engineering spin splitting in other materials.

Double Wall Cooling, Augmented Surface Heat Transfer & Transonic Turbine Blade Tip Heat Transfer

by Phil Ligrani, Member EUAS

Short Biography

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

PROFESSIONAL PREPARATION

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

APPOINTMENTS

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

ARCHIVAL JOURNAL PUBLICATIONS AND RELATED ITEMS.

As of December 2020, Dr. Ligrani is author or co-author of more than 197 publications in archival journals, including the International Journal of Heat and Mass Transfer, the ASME Transactions-Journal of Turbomachinery, the ASME Transactions-Journal of Engineering for Gas Turbines and Power, the ASME Transactions-Journal of Heat Transfer, the ASME Transactions-Journal of Fluids Engineering, Nature - Scientific Reports, the Journal of Fluid Mechanics, the AIAA Journal, Experiments in Fluids, Physics of Fluids, the AIAA Journal of Heat Transfer and Thermophysics, the International Journal of Rotating Machinery, Separation Science and Technology, Sensors and Actuators A: Physical, and the Journal of Microcolumn Separations. He is also author of 10 book chapters, and about 150 conference presentations and publications. A number of these are invited conference presentations at international meetings, at locations which include Korea, France, the Ukraine, Croatia, Germany, England-United Kingdom, and Belgium. From 1994 to 2020, he has also presented approximately 191 lectures at different institutions and establishments, including many invited lectures. From 2006 to 2020, he presented or is scheduled to present 7 Invited Keynote Papers, 12 Invited Papers, and 9 Invited Plenary Keynote Papers at different international conferences. Current SCOPUS Reference Citation H-INDEX is 44. Current GOOGLE SCHOLAR Reference Citation H-INDEX is 47.

EDITOR ACTIVITIES.

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

(CSA), and the China Aerodynamics Research and Development Center (CARDC), P. R. China (since 2018), (vii) Associate Editor, Energies Journal (since 2018), (viii) Associate Editor, ASME Transactions-Journal of Journal of Engineering for Gas Turbines and Power (2018-2021).

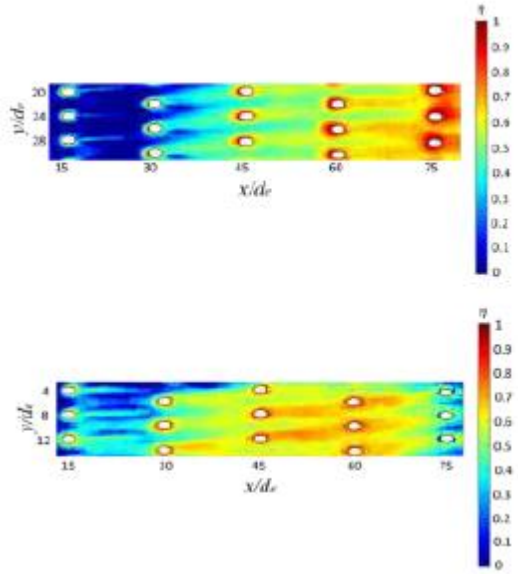
SELECTED RECENT HONORS, AWARDS, ACADEMIC RECOGNITIONS

● 2020 College of Engineering Outstanding Faculty Member Award. University Award, University of Alabama in Huntsville, Huntsville, Alabama, USA. ● 2020 Undergraduate Research and Creative Activity Mentor Award. University of Alabama in Huntsville, Huntsville, Alabama, USA. ● May 2020. Hermann Oberth Award in recognition of outstanding individual scientific achievement in the field of astronautics and advancement of the aeronautical sciences. AIAA – American Institute of Aeronautics and Astronautics. Greater Huntsville Section of the AIAA, Huntsville, Alabama, USA. ● March 2020. Employee Service Award, Five Years of Service. University of Alabama in Huntsville, Huntsville, Alabama, USA. ● ASME IGTI Outstanding Service Award 2019. ● 2019 University Distinguished Research Award for Excellence. University of Alabama in Huntsville, Huntsville, Alabama, USA. ● Outstanding Senior Faculty Member Award for 2019. College Award, College of Engineering, University of Alabama in Huntsville, Huntsville, Alabama, USA. ● Member. European Union Academy of Sciences (EUAS). 2019 to present. ● Guest Professor. School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai, P. R. China. 2019 to 2022. ● Outstanding Mechanical Engineer of the Year Award 2016, ASME – American Society of Mechanical Engineers, NAS - North Alabama Section, USA. ● Marquis Lifetime Achievement Award, Marquis Who's Who, New Providence, New Jersey, USA, 2016. ● Distinguished Advisory Professor, Inje University, South Korea, 2010 to 2022. ● Distinguished Lecture Award, 2011, CEAS Distinguished Lecture Series, College of Engineering, University of Wisconsin, Milwaukee, Wisconsin, USA. ● Distinguished Editorial Review Board membership for Springer Publishing Corporation. ● Carl E. and Jessie W. Menneken Faculty Award for Excellence in Scientific Research. ● NASA Space Act Tech Brief Award for "Development of Subminiature Multi-Sensor Hot-Wire Probes." ● Silver Winner for the Annual 26th Educational Advertising Awards for the Higher Education Marketing Report.

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

DOUBLE WALL COOLING RESEARCH INVESTIGATIONS

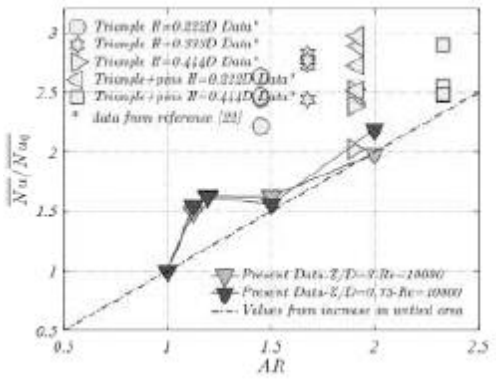
Provided are new effusion cooling data for both surfaces of full coverage effusion cooling plate. For the effusion cooled surface, measured are spatially-resolved distributions of surface adiabatic film cooling effectiveness, and surface heat transfer coefficients (measured using transient techniques and infrared thermography). For the impingement cooled surface, measured are spatially-resolved distributions of surface Nusselt numbers (measured using steady-state liquid crystal thermography). Recent research considers comparisons of hot-side effusion plate results for a mainstream flow passage with CR=1 (to provide a mainstream flow with zero streamwise pressure gradient) and for a mainstream flow passage with CR=4 (to provide an accelerated mainstream flow with favorable streamwise pressure gradient). The resulting variations of surface adiabatic film cooling effectiveness and surface heat transfer coefficients are due to three competing phenomena, including increased turbulent mixing and transport result from effusion coolant jets, decreased magnitudes of local blowing ratio with streamwise location, and significant streamwise acceleration, which induces local boundary layer re-laminarization. The attached figure shows that, when the CR=4 arrangement is employed (bottom figure part), these phenomena result in dramatic decreases of local adiabatic film effectiveness magnitudes, with streamwise development, relative to the CR=1 arrangement (top figure part), especially for x/d_e>60 at far downstream locations along the effusion cooled surface of the test plate.



AUGMENTED SURFACE HEAT TRANSFER USING TARGET SURFACES WITH SPECIAL SURFACE ROUGHNESS TEXTURES AND IMPINGEMENT JET ARRAYS.

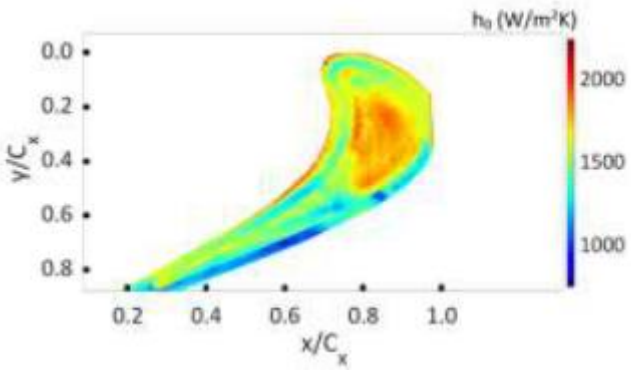
The combination of impingement jet arrays and target surface micro pin-fins often provides significant surface heat transfer augmentations. Considered are effects of varying jet to target plate distance, varying micro pin-fin shape, varying micro pin-fin height, and changing Reynolds number. For particular configurations and conditions, Nusselt number ratios show heat transfer augmentations, which generally increase as impingement jet Reynolds number increases, and are as high as 200 percent. Area-averaged Nusselt number variations for the different data sets are due to the effects of increased wetted surface area, turbulent transport and turbulent mixing caused by micro pin-fin elements, thermal conduction resistance from pin-fin material, and local flow separations and recirculation regions which are generally present just downstream of individual

roughness elements. Of particular importance are Reynolds number effects and significantly different area-averaged Nusselt number ratio behavior as surface roughness element height is changed. A results example is shown within the attached figure with area-averaged Nusselt number ratio variation with wetted area ratio.



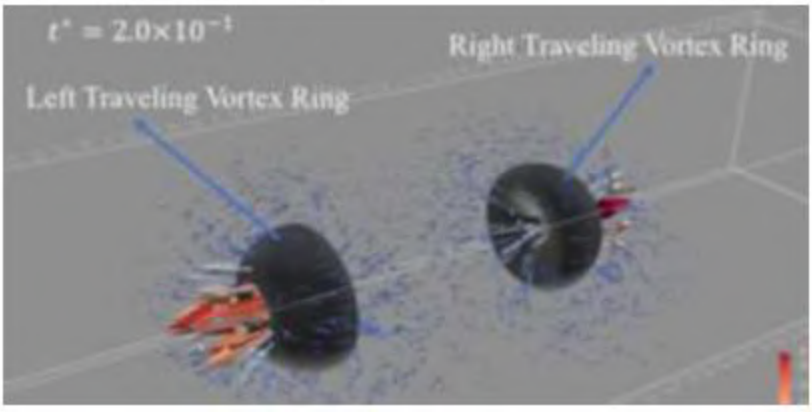
TRANSONIC TURBINE BLADE TIP HEAT TRANSFER WITH INNOVATIVE FILM COOLING CONFIGURATIONS

Investigated are spatially-resolved distributions of surface adiabatic film cooling effectiveness and surface heat transfer coefficients for a transonic turbine blade tip. Employed for the investigation is a two-dimensional linear cascade with four flow passages and five complete blades. Included within this facility are boundary layer flow bleed devices, and augmented cascade inlet turbulence intensity. The blade tip contains a squealer rim. A single row of film cooling holes is located on the pressure-side of the central blade very near to the blade tip. The cascade is designed to provide geometric similarity with the engine application environment, including inlet boundary layer thickness, blade configuration (including blade axial chord length, and blade true chord length), cascade arrangement (including blade pitch, blade span, and inlet flow angle), blade tip geometry, squealer depth, squealer wall thickness, and tip gap magnitudes. Surface heat transfer characteristics are measured using the transient impulse-response measurement approach, employed with infrared thermography. To create this arrangement, a step in mainstream temperature is provided after flow characteristics are established. With this approach, spatially-resolved distributions of surface adiabatic film cooling effectiveness and surface heat transfer coefficients are provided for different film cooling flow conditions. Results show that significant variations in surface thermal protection and film cooling coverage occur, as the blowing ratio varies, for different locations on the blade squealer tip, and on the upper pressure side of the blade, as evidenced by important local variations of surface heat transfer characteristics. An example of a measured distribution of baseline surface heat transfer coefficients is illustrated within the attached figure.



INVESTIGATIONS OF ELASTIC INSTABILITES AND ELASTIC TURBULENCE

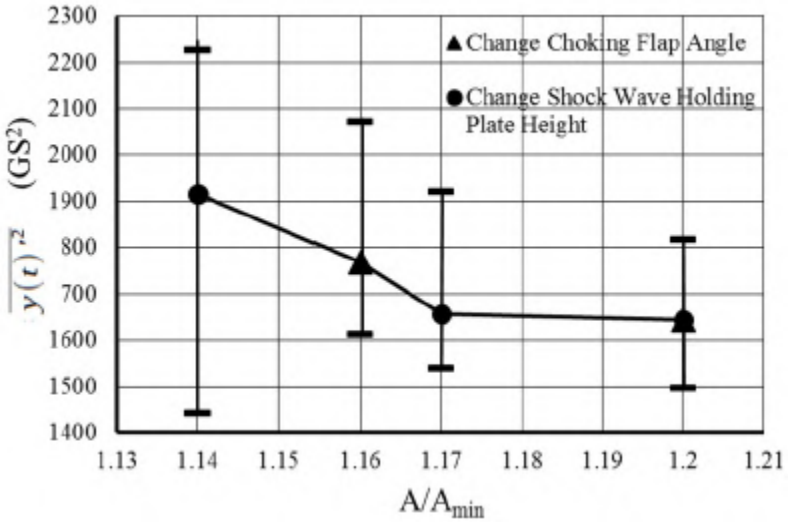
The remarkable ability of viscoelastic fluids to augment local and global thermal transport and surface heat transfer characteristics is demonstrated by experimental results, provided for a Rotating Couette Flow (RCF) environment with convective heat transfer. Augmented surface Nusselt numbers are measured for sucrose-based, viscoelastic solutions with polyacrylamide (as they are subject to different magnitudes of flow strain), relative to Newtonian flows and relative to fluids with zero shear rate. Nusselt numbers are as high as 3.0 for the highest polymer concentration and highest shear shear rate considered, whereas zero shear rate values are in the vicinity of 1.0. These enhancements are associated with the onset and development of elastic instabilities, which show that the Weissenberg number is the parameter which best correlates and characterizes Nusselt number augmentations. Numerical and analytic results, using a finitely extensible nonlinear elastic Peterlin (FENE-P) model, demonstrate the existence of clearly identifiable vortical structures (e.g. vortex rings) which are generated by the release of elastic stresses. Such vortex motions in turn promote bulk mixing, since such motions transport fluid elements from one location to another more efficiently than diffusion alone. The attached figure shows a visualization of the three-dimensional velocity vector field associated with vortex rings formed by the release of elastic energy. Iso-surfaces of the vorticity magnitude visualize the right and left traveling vortex rings. Each vector within this figure is color coded according to its magnitude.



CONTROL OF SHOCK WAVE STRUCTURE AND UNSTEADINESS

Despite over fifty years of research on shock-wave-boundary-layer-interaction unsteadiness, the source, origin, and propagation direction of the unsteadiness remains controversial and a debated

topic. The present research effort is designed to address normal shock wave unsteadiness characteristics, using a newly-developed, supersonic wind tunnel, which is located at the University of Alabama in Huntsville, USA. The wind tunnel test section includes a two flow passage arrangement, where each passage is separated by a shock wave holding plate. The top wall for the top passage is contoured relative to the streamwise flow direction, and a choking flap is located at the downstream portion of the bottom flow passage. With this arrangement, the Mach number at the test section inlet is 1.54, and total air mass flow rate is approximately 12.5 kg/s. Of particular interest are spatially- and temporally-varying flow structural characteristics, which are quantified using shadowgraph flow visualization images, grayscale value spectral energy variations, magnitude squared coherence variations with frequency, and time lag magnitude variations with frequency, where these last two quantities are determined for different flow locations relative to shock wave locations. The attached figure shows overall, integrated magnitudes of spectral energy associated normal shock wave unsteadiness. Such data illustrate how shock wave unsteadiness is controlled, using different test section bottom passage area ratios, as the height of the shock wave holding plate is altered and as the choking flap angle is altered. Overall, results from the present parametric investigation show that shock wave location and orientation are related to the local variation of static pressure ratio, and to passage area ratio variations, provided static and stagnation pressures are approximately constant at the inlet of the test section. As static pressure ratios within the bottom flow passage increase, shock waves generally become more normal as they are positioned farther upstream. This occurs either by (a) increasing choking flap angle, (b) decreasing the amount of venting from the exhaust plenum, or (c) decreasing the height of the shock wave holding plate from the centerline of the test section.



On the Symbiosis between our Two Interacting Brains

by Alain L. Fymat, Member EUAS

Short Biography

DR. ALAIN L. FYMAT is a medical-physical scientist and an educator. He is the current President/ CEO and Institute Professor at the International Institute of Medicine & Science with a previous appointment as Executive Vice President/Chief Operating Officer and Professor at the Weil Institute of Critical Care Medicine, California, U.S.A. He was formerly Professor of Radiology, Radiological Sciences, Radiation Oncology, Critical Care Medicine, and Physics at several U.S. and European Universities. Earlier, he was Deputy Director (Western Region) of the U.S. Department of Veterans Affairs (Office of Research Oversight). At the Loma Linda Veterans Affairs Medical Center, he was Scientific Director of Radiology, Director of the Magnetic Resonance Imaging Center and, for a time, Acting Chair of Radiology. Previously, he was Director of the Division of Biomedical and Biobehavioral Research at the University of California at Los Angeles/Drew University of Medicine and Science. He was also Scientific Advisor to the U.S. National Academy of Sciences, National Research Council, for its postdoctoral programs tenable at the California Institute of Technology and Member of the Advisory Group for Research & Development, North Atlantic Treaty Organization (NATO). He is Health Advisor to the American Heart & Stroke Association, Coachella Valley Division, California. He is a frequent Keynote Speaker and Organizing Committee member at several international scientific/medical conferences. He has lectured extensively in the U.S.A, Canada, Europe, Asia, and Africa. He has published in excess of 500 scholarly scientific publications and books. He is also Editor-in-Chief, Honorable Editor or Editor of numerous medical/scientific Journals to which he regularly contributes. He is a member of the New York Academy of Sciences and the European Union Academy of Sciences, a Board member of several institutions, and a reviewer for the prestigious UNESCO Newton Prize, United Kingdom National Commission for UNESCO.

RESEARCH INTERESTS

*Dr. Fymat's current research interests are focused on neurodegenerative diseases (Alzheimer's, Parkinson's, dementias, epilepsy, and others), oncology (glioblastoma), epigenetics & ecogenetics, and nanomedicine & nanobiotechnology. These are represented in part in his latest books: "**From the Heart to the Brain**: My collected works in medical science research (2016-2018)", "**Alzhei ...Who?** Demystifying the disease and what you can do about it", "**The Odyssey of Humanity's Diseases:** Epigenetic and ecogenetic modulations from ancestry through inheritance, environment, culture and behavior**"** Volumes 1, 2, and 3, "**Parkin..ss..oo..nn**: Elucidating the disease and what you can do about it", "**Lyme disease:** The great invader, evader, and imitator", "**Dementia:** Fending-off the menacing disease... and what you can do about it", and "**The Human Brain: Wonders and disorders:** My collected works in neuroscience research (2018-2020)".*

On the symbiosis between our two interacting brains

Evolutionarily, since times immemorial, humans have lived and continue to live in a permanent symbiotic relationship with the commensal indigenous microbial communities living within them, forming an integrated ecosystem. The gut microbiome, in particular, is known to affect the host's physiology in health and disease. Disruptions in its balanced composition (so-called "dysbiotic states") can be correlated with neurodegenerative disorders such as Alzheimer's, Parkinson's, and other such diseases, contributing to or modulating their etiology(ies) but *not* being their cause(s). Connecting the two brains (the brain-under-the-skull and the brain-in-the-gut) is the gut-brain axis along which bidirectional communication takes place. This communication is mediated by neurons (vagal afferent, spinal sympathetic), immune pathways, the hypothalamic-pituitary-adrenal axis, and metabolic mechanisms.

Having traveled along these communication pathways, bacteria, viruses, fungi, and other microbes are part of a growing list of pathogens found in the brains of patients with neurodegenerative diseases. Microbes in the brain may indicate meningitis or encephalitis, two diseases that are active infections with inflammation. However, for diseases like Parkinson's, Alzheimer's, and other like diseases that were not thought to be infectious, finding pathogens in the brain is both surprising and concerning. But, how do these organisms, and others, get into the brain since it is protected by the blood-brain barrier? They do so when the barrier is disrupted and looses some of its impermeability. Other avenues for reaching directly the brain are (a) the intra-nasal and sinus access, (b) the mouth (through the lingual nerve, which runs down the jawline and into the tongue), (c) the eye (through the olfactory bulbs), and, importantly here, (4) the gut (through the vagus nerve, which travels through the neck and thorax to the stomach), all of which connect to the brain by replicating and spreading.

The pathogen-brain connection is not a recently discovered one. It has been reported since before the mid-19th century and continues to this day. To summarize, in 2003**,** Heiko Braak proposed that Parkinson's disease starts in the gut, then, moves into the brain in a process that may take place over 25-30 years of life of the infected individual. In 2008, in ducks infected by the H5N1 virus, Smeyne and his collaborators wondered whether a connection existed between the viral infection and the extensive neurodegeneration they observed (namely, the devastation of the *substantia nigra*, which is often damaged in Parkinson patients, and the obliteration of all neurons). In people infected with H5N1, the symptoms are inflammation of the brain that leads to tremors and other motor malfunctions, which is Parkinsonism, involving only a subset of the disease's symptoms. In sum, the virus induced inflammation and death into those parts of the brain that degenerate in Parkinson's. Rejoining the Braak hypothesis, Smeyne also suggested a possible pathway for the virus to spread from the body into the brain by infecting neurons first in the gut, then into the vagus nerve, and subsequently into the *substantia nigra*. Still further, he remarked that in rodents, which have a much shorter lifetime than humans, the same travel from the gut to the brain may take only a few weeks as opposed to decades in humans. Even if they cannot reach the brain, the viruses can still play a role in neurodegeneration by triggering severe inflammation. In 2009, in mice, Smeyne also observed that H5N1 not only is not blocked by the blood-brain barrier from entering the brain but it can easily infiltrate nerve cells in the brain and kill them, especially targeting the dopamine-

producing neurons in the *substantia nigra.* Further, while H1N1 could not penetrate the barrier, it still caused central nervous system immune cells (the microglia) to flow into the *substantia nigra* and the hippocampus, causing inflammation and cell death in the area. Interestingly, we have here two different flus, two different mechanisms, but the same effect! Inflammation and death are induced in that part of the brain that degenerates in Parkinson's disease.

It must be noted that Smeyne's experiments are not the only ones to suggest that viral infections can contribute to neurodegenerative diseases, and the connection is not limited to influenza. Several different viruses, including measles and herpes can give rise to symptoms of multiple sclerosis in rodents. Also, levels of herpes virus are higher in the brains of people who died from Alzheimer's than in those without the disease. Further, some HIV patients develop dementia that appears to be associated with the infection. Later, in 2017, after administering the toxin MPTP, a byproduct of a bad batch of synthetic heroin that led users to develop Parkinson's, Smeyne observed that the treated mice developed signs of Parkinson's and lost 25% more neurons in the *substantia nigra* than uninfected mice treated with the toxin. He, then, concluded that whereas the H1N1 viral infection alone may not cause Parkinson's, it primed the nervous system to be sensitive to other things that would.

Notwithstanding these several instances of the link between viruses and neurodegenerative diseases, particularly along the gut-brain axis, I had concluded that they remain correlations or contributions, but *not* causes of the diseases. I further posited that these diseases are but the manifestation of a runaway autoimmune disease.

On another front, the enteric nervous system consists of sheaths of neurons embedded in the walls of our alimentary canal. It likely evolved to perform digestion and excretion "on-site," rather than remotely from our brain. Filled with important neurotransmitters (it uses more than 30 neurotransmitters, just like the brain), it handles much more than mere digestion. About 90% of the fibers in the primary visceral nerve (the vagus) carry information from the gut to the brain and not the other way around.

The second brain (the brain-in-the-gut) contains some 100 million neurons, more than in either the spinal cord or the peripheral nervous system. This multitude of neurons enables us to "feel" the inner world of our gut and its contents. Much of this neural firepower comes to bear in the elaborate daily grind of digestion: breaking down food, absorbing nutrients, and expelling waste, requiring chemical processing, mechanical mixing, and rhythmic muscle contractions to move everything on down the line.

In connection with our primary brain, our second brain determines our mental state and plays key roles in certain diseases throughout the body. However, despite its far-reaching influence, the second brain is not the seat of any conscious thoughts or decision-making process. Equipped with its reflexes and senses, it can control gut behavior independently of the brain. It also informs our state-of-mind in other more obscure ways in that a big part of our emotions is probably influenced by the nerves in our gut, for example, “butterflies” in the stomach signal our physiological stress response, gastrointestinal turmoil can sour one's moods, etc. Everyday emotional well-being may rely on messages from the brain below to the brain above. For example, electrical stimulation of the vagus nerve—a useful treatment for depression—may mimic these signals so that other depression treatments that

target the mind can unintentionally impact the gut. Another example is provided by our body's serotonin ~95% of which is found in the bowels. Because antidepressant medications called selective serotonin reuptake inhibitors increase serotonin levels, it is little wonder that medications meant to cause chemical changes in the mind often provoke gastrointestinal issues as a side effect. Irritable bowel syndrome, which arises in part from too much serotonin in our entrails, could perhaps be regarded as a "mental illness" of the second brain. Serotonin seeping from the second brain might also play a role in counteracting several other diseases, including osteoporosis (the bone-deteriorating disease in postmenopausal women) and autism (the developmental disorder often first noticed in early childhood, explaining why so many kids with autism also have gastrointestinal motor abnormalities). In the same way that connections between the brain and spinal cord lesions indicate multiple sclerosis, I conjecture that connections between diseases and lesions in the gut's nervous system may be found. Further, since at least 70% of our immune system is aimed at the gut to expel and kill foreign invaders, the second brain may be mediating the body's immune response – a immensely interesting observation.

The brain under-our-skull (a part of our central nervous system) and the one in-our-gut (a part of the intrinsic or enteric nervous system) re in constant communication. How do they do it? Until recently, we thought the two systems communicated solely via enteroendocrine cells scattered throughout the gut's lining. When stimulated, these cells release hormones that either enter the bloodstream or activate nearby nerves to stimulate appetite. The sensory signal from a nutrient is transformed into an electrical signal that alters behavior. Endowed with microvilli (or tiny protrusions exposed to the gut) but also a foot-like extension (called a "neuropod"), enteroendocrine cells have similar physical attributes to neurons and might be wired to them. Some make physical contact with the enteric nervous system, forming synapses with nerves. Beyond the gut, the linings of our body's organs (lungs, prostate, and vagina) all possess sensor cells similar to enteroendocrine cells. The brain perceives signals from these organs and affects our reactions to them.

Charting the gut-brain axis communication pathway could someday lead us to new treatments for non-neurodegenerative diseases including autism, inflammatory bowel disease, irritable bowel syndrome, obesity, and even disorders once thought to be solely psychological such as anorexia, chronic stress, and post-traumatic stress disorder.

In summary, our two brains (brain above, brain below) communicate bi-directionally through the gut-brain pathway (or axis). Dysbiotic states of the gut microbiome can be correlated with neurodegenerative diseases, contributing to or modulating their etiology(ies) but *not* being their root cause(s). Effects on neurodegenerative and gastroenteric diseases have been shown. Examples include Parkinson's and Alzheimer's disease, effects of certain antidepressant medications (selective serotonin reuptake inhibitors) meant to cause chemical changes in the mind showing gastrointestinal side effects, irritable bowel syndrome, osteoporosis (the bone-deteriorating disease in postmenopausal subjects), and developmental disorders (such as autism). In the same manner that connections between the brain and spinal cord lesions indicate multiple sclerosis, connections between the gut and enteric nervous system lesions may explain gastroenteric diseases. Cutting-edge research is currently investigating how the second brain also mediates the body's immune response.

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Renin – Angiotensin - Aldosterone System Blockers and the Risk of Covid-19

by Giuseppe Mancia, Member EUAS

Short Biography

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

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

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

SCIENTIFIC SOCIETES/TASK FORCES/COMMITTEES. *GM has served as Member of the Scientific Council, Secretary and President of the International Society of Hypertension (ISH) between 1982 and 1992, President of the European Society of Clinical Investigation (1980-1982), Chairman of the Working Group on Hypertension and the Heart of the European Society of Cardiology (ESC,1994-1996), member of the Executive Scientific Committee of ESC (1986-1991), President of the Italian Society of Hypertension (1997-1999) and member of the Scientific Council of ESH between 1989 and 2003 (President, 1999-2001). He has been member ex-officio (only European) of the Executive Council of the American Society of Hypertension (1996-2008), Officer for the ISH Forum of National Societies, member of the Committee on Cardiovascular Drugs and Therapy of the World Heart Federation and member of the Writing Committee of the ESC guidelines on Prevention of Cardiovascular Diseases (1993, 1998, 2003),the WHO/ISH Guidelines on Hypertension (1993, 1999) and the Guidelines on Hypertension in the Elderly of the American College of Cardiology (2011).He has co-chaired the Task Force on the ESH-ESC guidelines on Hypertension (2003,2007,2009 and 2013 and 2018) and the WHO/ISH Liaison Committee. He has chaired the Scientific and Organising Committees of various ESH Meetings (2001, 2003, 2005, 2007, 2009, 2011, 2013,2015,2017 and 2019). He has been Chairman of the Scientific Committee of the ISH Congresses in Prague (2002) and San Paulo (2004), and Honorary President of the ISH Meeting in Montreal (1990), Athens (ESH/ISH meeting,2014) and Glasgow (ESH/ISH Meeting, 2020).He is currently Chairman of the Educational Board of ESH.*

AWARDS/HONORS. *GM has received several Awards, among which the AHA Award for Excellence in Hypertension Research, the Heymans Award of the International Society of Pharmacology, the Wright International Award of the High Blood Pressure Council of Australia, the ISH Volhard and the Tigersted (MSD) Awards, the ESH Folkow Award, the Life Achievement Award of the Italian Society of Hypertension, the Peter Sleight Award of the World Hypertension League and the Alberto Zanchetti Life Achievement Award of ESH. He was appointed Lecturer of the Year by the Belgian Universities and Hypertension Leagues (1992) and was conferred the Talal Zein Foundation Award, the International Recordati Prize (2000), the 2001 Invernizzi Award for Medicine, the Gold Medal of the Lorenzini Foundation (2008),the Hariri Memorial Award (2009) and the Spinoza Award of the Amsterdam University.He has been appointed Honorary Member of ESH, the High Blood Pressure Council of Australia, the Latino-American Hypertension Society and the Japanese Circulation Society. He is honorary member of other Scientific Academies or Societies, among which the British Hypertension Society, the German Hypertension League and many national Hypertension or Cardiology Societies . He has received the highest Award of the Lombardy Region (Rosa Camuna) and the title of Commander of the Order of the Italian Republic. He has recently been awarded as one of the 100 Italian excellences in various areas of human activities.*

He is member of the European Academy of Sciences
He has been invited to give state-of-the-art, keynote, debates or special and plenary lectures in more than 700 international meetings. He has also been guest lecturer at meetings of many national societies of hypertension, cardiology awarded as one and internal medicine, among which the Pickering Lecture (British Hypertension Society), the Tigersted Lecture (Finnish Hypertension Society), the Merck Frosst Lecture (Canadian Society of Cardiology), the Saeb Salam Memorial Lecture (Beirut University), the Brian Bronte Steward Memorial Lecture (Glasgow University) the Leloir Nobel Laureate Lecture (Buenos Aires),the Mac Donald Lecture (Hamilton),the Gavras Life Achievement Award Lecture (Athens),and the Population Health Lecture (Mac Master University, Hamilton).
***HONORARY DEGREES/ACADEMIC RECOGNITIONS**. GM has received the Honorary Professorship of the University of Cordoba. He is Honorary member of the Academy of Science of Cordoba, and has been conferred the Degree Honoris Causa in Medicine from the University of Gdansk and the Carol Davila University of Bucharest. He has also received the Degree Honoris Causa (Doctor of Science) from the University of Glasgow.*
***EDITORIAL ACTIVITY**. GM has edited more than 90 Special issues or Supplements to international cardiovascular and internal medicine Journals. He has written or edited more than 20 books on hypertension, metabolic diseases and cardiovascular diseases edited by international Publishers, among which several Manuals, including the official ones of ESH. He is or has been member of the Editorial Board, Guest Editor and Reviewer of many important international journal on hypertension, cardiovascular disease and internal medicine. He is Editor-in-Chief of the Journal of Hypertension, the official ISH/ESH Journal.*
***SCIENTIFIC ACTIVITY**. GM's research interests focus on epidemiology pathophysiology, diagnosis and treatment of hypertension, heart failure, and coronary disease, as well as on the clinical aspects of diabetes, obesity and other metabolic abnormalities. His expertise includes ambulatory blood pressure monitoring, neurohumoral control of the circulation, large artery mechanics, cardiac damage in hypertension, hemodynamic changes of cardiovascular drugs, cardiovascular regulation during stress and sleep as well as epidemiology and intervention trials in hypertension and diabetes. He has been member or chairman of the steering committees of several clinical trials. He has published more than 2000 original papers, reviews and editorials in peer-review journals.*
***BIBLIOMETRIC DATA**. GM is since many years in the list of the Highly Cited scientists (Thomson Reuters) . One of his papers (2003 ESH/ESC Guidelines) has been the most highly cited article in the world medical literature in the years 2004-2005 (Ref. The Scientist) and three have been included among the most widely quoted hypertension papers ever (Ref. Hypertension,2014).In 1995 he was classified as the most widely quoted cardiologist in Italy and in 2013 has been included among the 400 most influential biomedical investigators in the world (Ref. Eur J Clin Inv,Scopus 1996-2011).In 2019 he has been classified as the first expert in Europe and the second in the world for the area Hypertension-Cardiovascular for the 2008-2018 publications (ref. Expertscape). Recently, an assessment of about 6 million scientists and 7 million papers from 22 research areas (Ref. Plos Biology)has ranked him among the 250 scientists in the world as well as the 12th world cardiologist and 1st hypertensiologist. GM's publications have received, up to August 2020, more than 217.000 citations in the international medical literature, with a H-index of 178 (Ref. Microsoft Academy), the highest among Italian cardiologists and internists.*

Renin-Angiotensin-Aldosterone System Blockers and the Risk of Covid-19.

Giuseppe Mancia, Federico Rea, Monica Ludergnani, Giovanni Apolone, Giovanni Corrao

Abstract

Background: A potential association between the use of angiotensin-receptor blockers (ARBs) and angiotensin-converting-enzyme (ACE) inhibitors and the risk of coronavirus disease 2019 (Covid-19) has not been well studied.

Methods: We carried out a population-based case-control study in the Lombardy region of Italy. A total of 6272 case patients in whom infection with severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) was confirmed between February 21 and March 11, 2020, were matched to 30,759 beneficiaries of the Regional Health Service (controls) according to sex, age, and municipality of residence. Information about the use of selected

drugs and patients' clinical profiles was obtained from regional databases of health care use. Odds ratios and 95% confidence intervals for associations between drugs and infection, with adjustment for confounders, were estimated by means of logistic regression.

Results: Among both case patients and controls, the mean (±SD) age was 68±13 years, and 37% were women. The use of ACE inhibitors and ARBs was more common among case patients than among controls, as was the use of other antihypertensive and non-antihypertensive drugs, and case patients had a worse clinical profile. Use of ARBs or ACE inhibitors did not show any association with Covid-19 among case patients overall (adjusted odds ratio, 0.95 [95% confidence interval {CI}, 0.86 to 1.05] for ARBs and 0.96 [95% CI, 0.87 to 1.07] for ACE inhibitors) or among patients who had a severe or fatal course of the disease (adjusted odds ratio, 0.83 [95% CI, 0.63 to 1.10] for ARBs and 0.91 [95% CI, 0.69 to 1.21] for ACE inhibitors), and no association between these variables was found according to sex.

Conclusions: In this large, population-based study, the use of ACE inhibitors and ARBs was more frequent among patients with Covid-19 than among controls because of their higher prevalence of cardiovascular disease. However, there was no evidence that ACE inhibitors or ARBs affected the risk of COVID-19.

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Limited reproducibility of MUCH and WUCH: evidence from the ELSA study.

Giuseppe Mancia, Rita Facchetti, Cesare Cuspidi, Michele Bombelli, Giovanni Corrao, Guido Grassi

Eur Heart J 2020 Apr 21;41(16):1565-1571.
doi: 10.1093/eurheartj/ehz651.

Abstract

Aims: To evaluate the long-term reproducibility of masked (MUCH) and white-coat uncontrolled hypertension (WUCH), an information crucial for determining the long-term prognostic impact of these conditions.

Methods and results: Reproducibility of MUCH and WUCH was assessed in 1664 hypertensive patients recruited for the European Lacidipine Study on Atherosclerosis and treated with atenolol or lacidipine (±additional drugs) during a 4-year period. Office and 24 h blood pressure (BP) was measured at baseline and every year during treatment, allowing repeated classification of either condition. After 1 year of treatment 21.1% and 17.8% of the patients were classified as MUCH and WUCH, respectively. For both conditions the prevalence was similar in the following years, although with a large change in patients composition because only about 1/3 of patients classified as MUCH or WUCH at one set of office and ambulatory BP measurements maintained the same classification at a subsequent set of measurements. In only 4.5% and 6.2% MUCH and WUCH persisted throughout the treatment period. MUCH and WUCH reproducibility was worse than that of patients showing control or lack of control of both office and ambulatory BP, i.e.

controlled and uncontrolled hypertension, respectively.

Conclusion: Both MUCH and WUCH display poor reproducibility over time. This should be taken into account in studies assessing the long-term prognostic value of these conditions based on only one set of BP measurements.

Antihypertensive Treatment in Elderly Frail Patients: Evidence From a Large Italian Database.

Federico Rea, Anna Cantarutti, Luca Merlino, Andrea Ungar, Giovanni Corrao, Giuseppe Mancia

Hypertension 2020 Aug;76(2):442-449.
doi: 10.1161/HYPERTENSIONAHA.120.14683. Epub 2020 Jun 8.

Abstract

Aim of our study was to assess the relationship between adherence with antihypertensive drugs and the risk of death in frail versus nonfrail old individuals. Using the database of the Lombardy Region (Italy), we identified 1 283 602 residents aged ≥65 years (mean age 76) who had ≥3 prescriptions of antihypertensive drugs between 2011 and 2012. A nested case-control design was applied, with cases being the cohort members who died during the observation period (7 years). Logistic regression was used to model the association of interest, with adjustment for potential confounders. Adherence was measured by the proportion of the follow-up covered by prescriptions, and the analysis was separately performed in patients with a good, medium, poor, and very poor clinical status, as assessed by a score that has been shown to be a sensitive predictor of death in the Italian population. The 7-year death probability increased from 16% (good) to 64% (very poor) clinical status. Compared with patients with very low adherence with antihypertensive treatment (<25% of follow-up time covered by prescriptions), those with high adherence (>75% of time covered by prescriptions) exhibited a lower risk of all-cause mortality in each group, the difference decreasing progressively (-44%, -43%, -40%, and -33%) from the good to the very poor clinical status. Adherence with antihypertensive drug treatment was also associated with a lower risk of cardiovascular mortality. Adherence with antihypertensive appears to be protective in frail old patients, but the benefit is less marked than in patients with a good clinical status.

Beta-blockers in hypertension: overview and meta-analysis of randomized outcome trials.

Costas Thomopoulos, George Bazoukis, Costas Tsioufis, Giuseppe Mancia

J Hypertens 2020 Sep;38(9):1669-1681

Abstract

Background: Meta-analyses from randomized outcome-based trials have challenged the role of beta-blockers for the treatment of hypertension. However, because they often

include trials on diseases other than hypertension, the role of these drugs in the choice of the blood pressure (BP)-lowering treatment strategies remains unclear.

Methods: Electronic databases were searched for randomized trials that compared beta-blockers vs. placebo/no-treatment/less-intense treatment (BP-lowering trials) or beta-blockers vs. other antihypertensive agents in patients with or without hypertension (comparison trials). Among BP-lowering trials and according to baseline comorbidity, we separately considered trials in hypertension, trials without chronic heart failure or acute myocardial infarction, and trials with either chronic heart failure or acute myocardial infarction. Seven fatal and nonfatal outcomes were calculated (random-effects model) for BP-lowering or comparison trials.

Results: A total of 84 BP-lowering or comparison trials (165 850 patients) were eligible. In 67 BP-lowering trials (68 478 patients; mean follow-up 2.5 years; baseline SBP/DBP, 136/82 mmHg), beta blockers were associated with a lower incidence of major cardiovascular events [risk ratio 0.85 and 95% confidence interval (95% CI) 0.78-0.92] and all-cause death (risk ratio 0.81 and 95% CI 0.75-0.86). Restriction of the analysis to five trials recruiting exclusively hypertensive patients (18 724 patients; mean follow-up 5.1 years; baseline SBP/DBP 163/94 mmHg), a -10.5/-7.0 mmHg BP decrease was accompanied by reduction of major cardiovascular events by 22% (95% CI, 6-34). In 24 comparison trials (103 764 patients, 3.92 years of mean follow-up), beta-blockers compared with other agents were less protective for stroke and all-cause death in all trials and in trials conducted exclusively in hypertensive patients (averaged risk ratio increase 20 and 6%, respectively, for both cases).

Conclusion: Compared with other antihypertensive agents, beta-blockers appear to be substantially less protective against stroke and overall mortality. However, they exhibit a substantial risk-reducing ability for all events when prescribed to lower BP in patients with modest or more clear BP elevations, and therefore can be used as additional agents in hypertensive patients.

Nanotechnology – Innovations & Applications

by Marcel Van de Voorde, Member EUAS

Short Biography

Studies at the Catholic University Leuven (B), University of Technology Delft (NL), Nancy University/School of Mines (F):

Industrial Engineer, Engineer in Chemistry, Physicist, Degree in Nuclear Engineering
PhD in Natural & Technical Sciences

Academic Career: now "Emeritus professor " (1975 - …)

** Professor University of Technology DELFT (NL)*
** Visiting & Honorary Professor: State University Ghent (BE), La Sapienza University(I), Cracow (PL), Columbia University (NY), Tsinghua University Beijing (China), Tokyo University (Japan)*

Scientific - Professional Career "Emeritus status "(1970 - …..)

Direction/Senior Research management functions:

** CERN (European Organisation for Nuclear Research), Geneva (CH), I*
** European Commission Research (B)*
** Distinguished Visiting Professor Max Planck Institute Stuttgart (D),*
** Science Council of the French Senate and National Assembly, Paris (F)*
** Co-Founder and Executive Advisor to CEO's & President of IMEC-Technology Institute*

(Former & Present: "Member, Chairman & President of Science Research Councils/Governing Boards (1975 - …)

****** *NATO & von KARMANN: Research & Technology, Brussels -Paris*
** ESA (European Space Agency), Hermes Programme, Noordwijk (NL) & Paris*
** CNRS (Conseil National pour la Recherche Scientifique), FR*
** CEA (Commissariat de l'Energie Atomique), FR*
** CNR (Consiglio Nazionale Delle Ricerche), IT*
** CSIC (Consiglio Superior de Investigaciones Cientificas), ES*
** JST (Japan Science& Technology), Tokyo – Japan*

The main topics and achievements in my career are summarized

40 years' experience in European & Worldwide Academic & Research & Innovative institutions: Professor – Scientist – Research manager – Director - Councillor.

** Disciplines: Physics: nuclear, low & high temperature, health; Polymer & Chemistry and Biochemistry, Materials & Aeronautics; Engineering; Medicine: Physical/medical imaging, Cancer treatment technology, Nanomedicine*

University professor at multiple Universities, worldwide:

- *Radiation chemistry, nuclear physics & engineering, radiation safety and protection*
- *High temperature materials for gas turbines for aeroengines and space applications*
- *Nanoscience and nanotechnology*

Research and technology:

- *Radiation damage studies, dosimetry, radiation chemistry, health physics*
- *Materials sciences. Metals, ceramics and polymers*
- *Nanoscience & nanotechnology: nanomedicine, nanoelectronics,*

- *Accelerator engineering*
- *Proton-therapy technologies for cancer treatments*

Spin-off technologies

- *Pioneering work in the foundation of IMEC – Leuven: institute where after 30 years existing 4.000 scientists/engineers/technicians from 100 different countries are employed.*

Promotion of University Education in Europe-active role in:

° The Ministerial Conference in Bologna – Uniformity of the Education throughout all European countries with the result of BSc, MSc and PhD programmes

° Pioneering work in the preparation on the EC: ERASMUS programme which lead to the mobility of students through Europe.

° The classification of Excellency of Universities in Europe has never been successful….a most critical subject which is still on the table.

Recent published science (study) books & encyclopaedia

**** Engineering, Medicine, and Science at the Nano-scale Study book for MSc and PhD students, WILEY Publ. Co November 2018; co-author with Prof. S. FONASH, PEN STATE University & Director US-NSF Nanoscience*

**** Nano cosmetics: SPRINGER Publ.in July 2019: co-authors Dr J. CORNIER & Prof. dr. Cornelia KECK*

**** Nanoscience and Nanotechnology: Advances and developments in Nano-sized Materials, DE GRUYTER Publ. Co June 2018*

**** Nanotechnology, Innovations & Applications.: Encyclopedia-15 Volumes WILEY Publ. Co in May 2017, series editor and author of chapters.: Nano Health Care, Nano Information and Communication, Nano Industry*

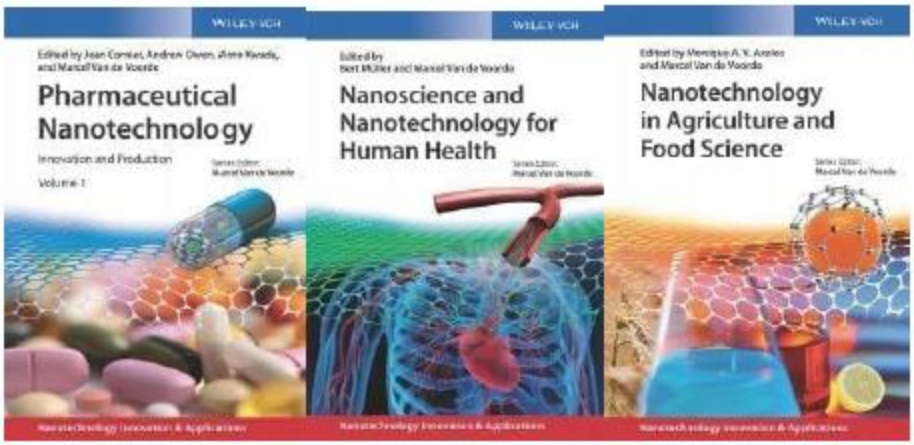
**** The Nano-Micro Interface, 2 Volumes WILEY publ. Co 2015 co-author with Prof. H.J. FECHT and Matthias WERNER*

**** Nanotechnology in a Nutshell, From Simple to Complex Systems, SPRINGER Publ. 2014 co-author with Dr C. NGO – CEA Paris*

**** GENNESYS White Paper: A new European partnership between nanomaterials science and technology and synchrotron radiation and neutron facilities, Max Planck Gesellschaft, 2011, Co-author with Prof. Dosch DG DESY (D)*

**** European White Book on Fundamental Research in Materials Sciences, Max Planck Institute, Stuttgart 2005, Co-author with MPI Colleagues*

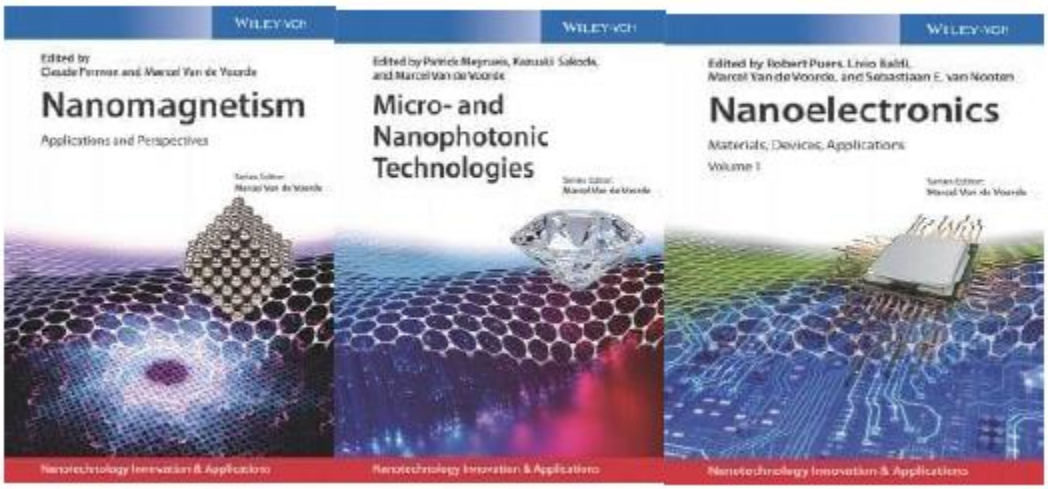
Human-Related Nanoscience and Nanotechnology



From medicine and pharmaceutical nanotechnology through nanoelectronics towards nanoenergy and industry: the new book series "Nanotechnology Innovation and Applications", published by Wiley-VCH, covers a broad spectrum of topics in nine subject-specific books.

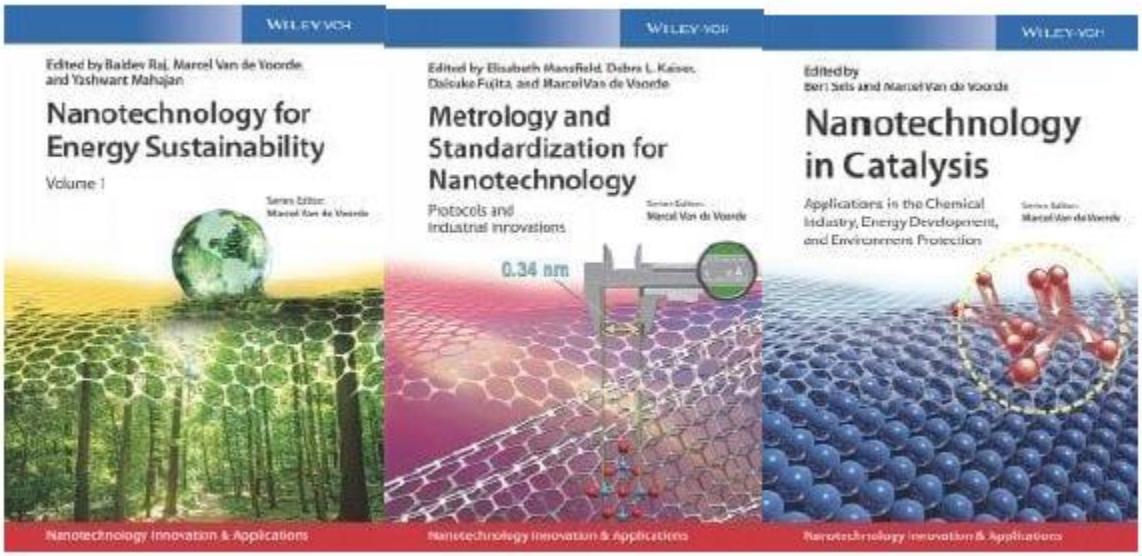
In recent years, nanoscience and nanotechnology have become particularly important technology areas worldwide. As a result, there are many universities that offer courses as well as degrees in nanotechnology.

Nanoscience and Nanotechnology in Information and Communication



Many governments including European institutions and research agencies have vast nanotechnology programs, and many companies file nanotechnology-related patents to protect their innovations. In short: nanoscience and nanotechnology are hot topics!

Nanoscience and Nanotechnology in Industry



Common to all the books in the series is that they represent top-notch research and are highly application-oriented, innovative and relevant for industry. A few numbers might illustrate the effort that went into the books in this series and the breadth of their coverage:

Altogether, there are 250 chapters, written by more than 500 authors, resulting in more than 6500 pages of content that is illustrated by more than 2200 figures and more than 300 tables.

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Publisher: WILEY-VCH: VERLAG GmbH KGaA – Heidelberg (D) - 2018 - 2020

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Prof. Dr. Dr. Marcel VAN DE VOORDE – Series Editor
Publisher: DE GRUYTER BERLIN – Berlin - Being published: 2021

Ethics in Nano-Technology

Prof. Dr. Dr. Marcel VAN DE VOORDE – Series Editor
Publisher: DE GRUYTER BERLIN – Berlin - Being published: 2021

Ultrasonic Transducer for Harsh Environment Applications with Bismuth Titanate Ceramic as Piezoelectric Element

by Bernhard R. Tittmann, Member EUAS

Short Biography

Schell Professor of Engineering, Emeritus
Director of Engineering Nanostructure Characterization Center
The Pennsylvania State University

Academic Training

B.S. (Physics and Mathematics), George Washington University, Washington, DC, 1957
Ph.D. (Solid State Physics), University of California at Los Angeles, CA, 1965

***Teaching Experience**:*

Professor, The Pennsylvania State University, University Park, PA 16802, 1989-present;
Visiting Professor, Fall 2017, University of California, Santa Barbara, CA
Visiting Professor, Spring 1995-1997. Johannes Kepler University, Linz, Austria.
Visiting Professor, University of Paris III, Physics Department, 1977, 1979, 1982.
Assistant Professor (in residence), 1965-1966. Physics Department, University of California at Los Angeles, CA.

Industrial Experience

Manager, Materials Characterization. Science Center, Rockwell Intern., 1979 - 1989.
Member Staff, Materials Mechanics Group. Science Center, Rockwell, 1966-1977.
Howard Hughes Fellow – Microwave Antenna Dept.; Hughes Research Lab., Culver City, CA, 1957-1962.

Professional Societies and Activities

American Ceramic Society (ACS), Member 1995 – present
American Society for Metals (ASM) International, Member 1993, Fellow 2006 – present
American Society of Nondestructive Testing (ASNT), Member 1980 – present
Materials Research Society (MRS), Member, 1995 – present
American Society of Mechanical Engineers (ASME), Member, 2001 – present
Acoustical Society of America (ASA), Fellow, 2001 – present
Technical Program Committee - Standing Member, 1999 to present
Institute of Electrical and Electronics Engineering (IEEE), Fellow, 1990 – present
Distinguished IEEE – UFFC Lecturer, June 1998 – December 1999
Vice-Chair of Awards Committee, IEEE – UFFC, 2003-present
International Society for Optical Engineering (SPIE), Senior Member

Awards/Honors

ASNT Research Council Award for Sustained Excellence 2019
National Academy of Inventors, Senior Member 2019
Albert Nelson Marquis Lifetime Achievement Award 2018
Top 100 Registry Professors of the Year, 2018
EU Academy of Sciences, 2018
Schell Professor, Emeritus 2017.
Endowed Chair at Penn State College of Engineering Schell Professor of Engineering 1989 (renewed 5 times) to June 2017.
IEEE-UFFC Distinguished Service Award 2017
IEEE-UFFC Invited Speaker at 2017 Int. Ultrasonics Symposium, Washington, D.C.
Named Consulting Editor of Archives of Acoustics, Polish Academy of Sciences, Warsaw, 2003
Penn State Engineering Society Outstanding Research Award, 1998

Senior Fulbright Fellowship, 1999
Rockwell Award for Highest IR&D Score Rockwell Science Center (1988)
NASA Principal Investigator Award for "Elastic and Anelastic Properties of Lunar Rock (1979)."
Howard Hughes Fellow (1957-1962).
Phi Beta Kappa (1957).
Graduation Cum Laude (1957).
G. Washington Tuition Scholarship (1953-1957).
Accomplishment
Graduated 11 PhD students and 25 MS students.
Citations 4969; h-index 35; i10 index 121
Nearly 500 publications including refereed journal publications and refereed Proceedings.
8 Patents

Ultrasonic Transducer for Harsh Environment Applications with Bismuth Titanate Ceramic as Piezoelectric Element - a Review.

Introduction

Ultrasonic transducers play a key role in many strategically important fields in health monitoring and nondestructive testing. Applications that use ultrasonic transducers include the medical, aerospace, railroad, marine, and energy-related industries. The heart of an ultrasonic transducer is the piezoelectric element. Transducers currently used in these industries primarily employ Lead-Zirconate-Titanate (PZT) as the piezoelectric element for ultrasound transmission and detection. This material is a ceramic which has a Curie–Weiss temperature that limits its use to below about 210 °C. Some industrial applications require much higher temperatures, i.e., a temperature range from 250 °C to as high as 1000 °C, depending on the application. Examples are heat engines, steam generators, heat exchangers, steam pipes, deep geological exploration, nuclear reactors, etc. Bismuth Titanate (BiTi) is a potential candidate for replacing PZT at the middle of the temperature range with many possible applications since it has a Curie–Weiss temperature of 685 °C.

The goal of this paper is to review Bismuth Titanate (BiTi) for use in harsh environments for the ultimate purpose of structural health monitoring (SHM), non-destructive evaluation (NDE), and material characterization (NDMC) with emphasis on materials testing in Nuclear Reactors in which typical temperatures are about 400 °C. Described are the results of a nuclear reactor experiment with an ultrasonic test capsule using BiTi as the piezoelectric element.

Bismuth Titanate, the material.

Bismuth Titanate is a member of the bismuth oxide layer structure ferroelectrics and has a perovskite crystal structure below the ferroelectric Curie temperature. It has the formula ($Bi_4Ti_3O_{12}$) and is a candidate for high-temperature piezoelectric applications because of its high Curie temperature of ~685^{O}C. It is also well known for its high dielectric constant, ~200 and highly anisotropic conductivity; its piezoelectric coefficients are d_{33} = 20 pC/N and K_{33} = 0.23.

Bismuth Titanate was discovered in 1949. Initially, the fabrication of bismuth titanate involved the conventional solid-state reaction processes, in which Bi_2O_3 and TiO_2 are mixed and then sintered at elevated temperatures. Since then, a variety of thin film techniques have been developed, such as physical vapor deposition, chemical vapor deposition, metal organic chemical vapor deposition and sol-gel.

Experiments

A. Temperature Tests

A test capsule with a piezoelectric transducer was fabricated with Bismuth Titanate (BiTi) as the active element (TRS Technologies BT-100). High purity aluminum foil was used to bond the BiTi sensor to a Kovar cylinder used as ultrasonic waveguide for a pulse echo operation. After the sensor was assembled, the assembly was heat treated at 610 °C to soften the foil and achieve better coupling to the waveguide as completed for the high temperature measurements.

First the Bismuth Titanate sensor was tested up to 650°C. The Bismuth Titanate sensor was capable of operating up to 550 °C. The pulse-echo amplitude experienced a significant increase in amplitude at 200 °C, rising as much as 250%. This amplitude was maintained until the transducer failed. Upon cooling of the sample-chamber the ultrasonic pulse echo amplitude returned to its pre-failure amplitude before a significantly decrease at 120°C. At the end of cooling the pulse-echo amplitude was not measurable. During reheating the pulse-echo amplitude increased back to its original amplitude, but on cooling its amplitude was significantly decreased. This was typical of the sensor for operation over several cycles.

B. Reactor Tests

Measurements were performed in the MIT (Massachusetts Institute of Technology) Reactor for 18 months. The transducer experienced an integrated neutron fluence of approximately 8.68 E + 20 n/cm^2 for n >1 MeV, temperatures in excess of 420 °C, and a gamma fluence of 7.23 Gy/cm^2. The BiTi transducer acoustically coupled to a Kovar cylinder gave acceptable pulse-echo data for most of the test. The BiT transducer was pulsed periodically using a commercial LabVIEW system. The transmitter/receiver sampled the sensor output at 1 GS/s for a period of 100 μs. The transmitter pulsed the sensor w a repetition rate of 1 kHz. A total of 256 measurements were averaged for each measurement. A total of 5038 measurements were made during the irradiation, with measurements being made every thirty minutes until the first power cycle, when the sensor was sampled every 2 hours.

The first waveform was acquired directly after the transducer was inserted into the reactor. There was significant ring down time from the main bang, taking between 10-15 μs to subside. There were several peaks in the Fast Fourier Transform (FFT) of the signal. There is a main through thickness resonant mode at 2.1 MHz, as well as up to 6 odd harmonics.

Fig. 1 shows a summary graph of the normalized ultrasonic pulse-echo amplitude and reactor power as function of the Fast Neutron Fluence during the entire 18 months operation. In these experiments, bismuth titanate operated up to a fast neutron fluence of 5E+20 n/cm^2. This was preceded by fairly large fluctuations in amplitude, as much as 20-40%. There was an initial decline in the amplitude of the fundamental harmonic starting on day 10 or at 1.28E+19 n/cm^2 and reaching a minimum relative amplitude of 60% at 5.29E+19 n/cm^2 on day 25. The amplitude gradually recovered to relative amplitude of 100% at 1.1E+20 n/cm^2. The sensor failure is noted by a significant decrease in the fundamental amplitude after 5E+20 n/cm^2. This decline occurred over a period of 17 days, dropping in amplitude by 80%. There was no notable recovery during this period;

however, an echo from the back wall of the waveguide was still measurable. At the end of the irradiation the DC impedance was measured to be 11 kΩ. Further, the piezoelectric coefficient d_{33} was 11.5±1.5 pC/N, measured from the drop-in sample after the irradiation. The d_{33} as reported by the material supplier, TRS Technologies, is 20 pC/N.

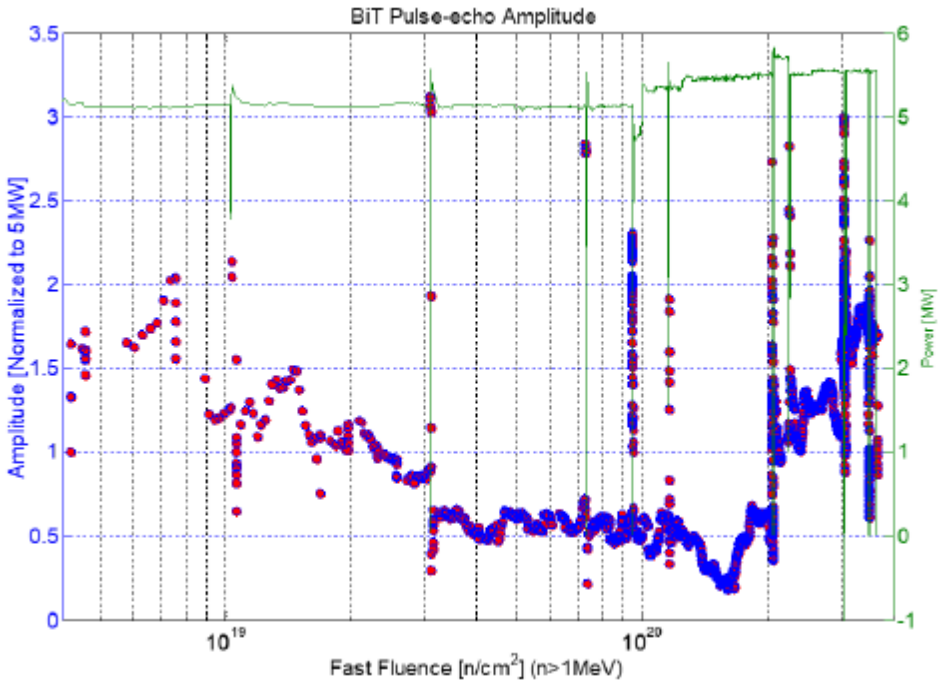

Figure 1: Pulse-echo amplitude of BiT sensor while in the reactor. The sudden drops in power correspond to down-times in the operation of the reactor output.

Summary

Ultrasonic methods offer the potential for Structural Health Monitoring of critical components in nuclear reactors. These efforts have been limited by ultrasonic transducers incapable of performance under high temperatures and/or irradiation conditions. Here we report on a piezoelectric transducer capsule designed, fabricated, tested and optimized to perform in harsh environments. The test capsule with piezoelectric transducers was fabricated with Bismuth Titanate (BiTi) as the active elements (TRS Technologies BI-100). Measurements were performed in the MIT Reactor for 18 months. The transducers experienced an integrated neutron fluence of approximately 8.68 E + 20 n/cm^2 for n >1 MeV, temperatures in excess of 420 °C, and a gamma fluence of 7.23 Gy/cm^2. The BiTi transducer acoustically coupled to a Kovar cylinder gave acceptable pulse-echo data for most of the test as shown in the summary of the test results. Thus, the feasibility of ultrasonic transducers in a nuclear reactor has been established and opens the door to leave-in-place sensors for in-reactor conditions and materials. [The authors gratefully acknowledge support from the Department of Energy under the ATR-NSUF program.]

Coordinate Indexing: On the use of Eulerian and Lagrangian Laplace Stretches

by Alan D. Freed, Member EUAS

Short Biography

Professor
J. Mike Walker '66 Department of Mechanical Engineering
Texas A&M University, College Station, TX 77843-3123, USA
Joint Faculty Appointment as a Mechanical Engineer
Impact Physics Branch, Protection Division, Weapons and Materials Research Directorate
Army Research Laboratory, Aberdeen Proving Ground, Aberdeen, MD 21005, USA

Education

PhD 1985 University of Wisconsin, Madison, WI, USA, Engineering Mechanics
minors Computer Science and Material Science
advisor Prof. Bela I. Sandor
committee Profs. Arthur S. Lodge, Millard W. Johnson, Jr., and Terry Richards
MS 1980 University of Wisconsin, Madison, WI, USA, Engineering Mechanics
BS 1978 University of Wisconsin, Madison, WI, USA, Engineering Mechanics

Employment

2018-present Joint Faculty Appointment, U.S. Army Research Laboratory, Aberdeen Proving Ground
2014-present Professor of Mechanical Engineering, Texas A&M University, TX, USA
2007-2014 Clifford H. Spicer Endowed Chair of Engineering, Saginaw Valley State University, MI, USA
2003-2007 Adjunct Staff, Lerner Research Institute, The Cleveland Clinic, Cleveland, OH, USA
1996-2007 Senior Research Engineer, NASA John H. Glenn Research Center, Cleveland, OH, USA
1989 Sabbatical at Office National d'Etudes et de Recherches Aérospatiales, Châtillon, Cedex, France. Mentored by Dr. Jean-Louis Chaboche
1985-1996 Research Engineer, NASA Lewis Research Center, Cleveland, OH, USA
1984-1985 Assistant Professor, Department of Mechanical Engineering, University of New Hampshire, USA
1978-1984 Graduate Teaching and Research Assistant, University of Wisconsin, Madison, WI, USA
1972-1974 Self-Employed Motorcycle Mechanic

Honors/Awards

2019 Member of the EU Academy of Sciences
2016 Brittan Undergraduate Teaching Award, Texas A&M University
2006 Cleveland Clinic Innovator Award
2004 NASA Exceptional Service Medal
2000 Fellow of the American Society of Mechanical Engineers (ASME)
1996 1996: NASA Superior Accomplishment Award

Journal Publications in 2020

Paul, S.*; Freed, A. D.; and Clayton, J. D.: "Coordinate indexing: On the use of Eulerian and Lagrangian Laplace stretches," *Applications in Engineering Science*, 5 (2021), 100029. DOI: 10.1016/j.apples.2020.100029.

Eulerian and Lagrangian measures for Laplace stretch are established, along with a strategy to ensure that these measures are indifferent to observer. At issue is a need to accommodate two invariant properties that arise as a byproduct of the Gram–Schmidt factorization procedure, which is used in the construction of these stretch tensors. Specifically, a Gram–Schmidt factorization of the deformation gradient implies that the 1 coordinate direction and the normal to the 12 coordinate plane remain invariant under transformations of Laplace stretch. The strategy proposed, which addresses these mathematical consequences, is that the selected 1 oordinate direction has minimal transverse shear, and that its adjoining 12 coordinate plane has minimal in-plane shear. From this foundation, a framework is built for the construction of constitutive equations that can use either the Eulerian or Lagrangian Laplace stretch as its primary kinematic variable.

Doehring, T.; Nelson, W.; Harris, T.; and Freed, A.: " FE vibration analyses of novel conforming meta-structures and standard lattices for simple bricks and a topology-optimized aerodynamic bracket," *Scientific Reports*, 10 (2020), 21484. DOI: 10.1038/s41598-020-78239-9

Additive manufacturing (AM) enables production of components that are not possible to make using traditional methods. In particular, lattice-type structures are of recent interest due to their potential for high strength-to-weight ratios and other desirable properties. However, standard periodic lattice structures have problems conforming to complex curved and multi-connected shapes (e.g. holes or sharp-to-smooth mating edges). In addition, standard lattices have well known shear and fatigue weaknesses due to their periodic basis/structure. To address these problems, we developed a new type of shape-conforming meta-structure (HGon) that extends lattices, enabling automated conforming to complex shapes and parametric meta-topology control. HGons also have unique vibration dampening and optimization capabilities. This study presents initial FE analyses of (Part 1) dynamic vibration responses of new HGon meta-structures compared with periodic lattices of equivalent density for a series of basic rectangular structures and (Part 2) a complex multi-connected aerodynamic bracket with field-based stress meta-topology optimization. Results show significantly enhanced vibration dampening behavior and superior strength-to-weight ratios for HGon meta-structures as compared to standard lattices.

Paul*, S.; and Freed, A. D.: "Characterizing Geometrically Necessary Dislocations Using an Elastic-Plastic Decomposition of Laplace Stretch," *Zeitschrift für angewandte Mathematik und Physik ZAMP*, 71 (2020), 196. DOI: 10.1007/s00033-020-01420-7

In this paper, the geometric dislocation density tensor and Burgers vector are studied using an elastic–plastic decomposition of Laplace stretch **U**. The Laplace stretch arises from a **QR** decomposition of the deformation gradient and is very useful, as one can directly and unambiguously measure its components by performing experiments. The geometric dislocation density tensor G is obtained using the classical argument of failure of a Burgers circuit in a suitable configuration κ_p where the deformation of a body is solely due to the movement of dislocations. The geometric features of space κ_p are explored. It is shown that the derived geometric dislocation tensor is related to the torsion of κ_p, which serves as a measure of incompatibility in this space. Additionally, G vanishes only when the space κ_p is compatible. A balance law for geometric dislocations is derived taking into account the effect of the dislocation flux and source dislocations. The physical meaning of the plastic Laplace stretch, and consequently, of the derived geometric dislocation tensor proves to be particularly useful in the classification of dislocations. Finally, the significance of the dislocation density tensor is discussed. The derived geometric dislocation density tensor could be specifically useful in developing a strain-gradient and size-dependent theory of plasticity.

Freed, A. D.; Zamani, S.*; Szabó, L.; and Clayton, J. D.: "Laplace stretch: Eulerian and Lagrangian formulations," *Zeitschrift für angewandte Mathematik und Physik ZAMP*, 71 (2020), 157. DOI: 10.1007/s00033-020-01388-4

Two triangular factorizations of the deformation gradient tensor are studied. The first, termed the Lagrangian formulation, consists of an upper-triangular stretch premultiplied by a rotation tensor. The second, termed the Eulerian formulation, consists of a lower-triangular stretch postmultiplied by a different rotation tensor. The corresponding stretch tensors are denoted as the Lagrangian and Eulerian Laplace stretches, respectively. Kinematics (with physical interpretations) and work-conjugate stress measures are analyzed and compared for each formulation. While the Lagrangian formulation has been used in prior work for constitutive modeling of anisotropic and hyperelastic materials, the Eulerian formulation, which may be advantageous for modeling isotropic solids and fluids with no physically identifiable reference configuration, does not seem to have been used elsewhere in a continuum mechanical setting for the purpose of constitutive development, though it has been introduced before in a purely kinematic setting.

Clayton, J. D.; and Freed, A. D.: "A Constitutive Framework for Finite Viscoelasticity and Damage based on the Gram-Schmidt Decomposition," *Acta Mechanica*, 231 (2020), 3319–3362. DOI: 10.1007/s00707-020-02689-5

A novel thermodynamic framework for the continuum mechanical response of nonlinear solids is described. Large deformations, nonlinear hyperelasticity, viscoelasticity, and property changes due to evolution of damage in the material are all encompassed by the general theory. The deformation gradient is decomposed in Gram–Schmidt fashion into the product of an orthogonal matrix and an upper triangular matrix, where the latter can be populated by six independent strain attributes. Strain attributes, in turn, are used as fundamental independent variables in the thermodynamic potentials, rather than the usual scalar invariants of deformation tensors as invoked in more conventional approaches. A

complementary set of internal variables also enters the thermodynamic potentials to enable history and rate dependence, i.e., viscoelasticity, and irreversible stiffness degradation, i.e., damage. Governing equations and thermodynamic restrictions imposed by the entropy production inequality are derived. Mechanical, thermodynamic, and kinetic relations are presented for material symmetries that reduce to cubic or isotropic thermoelasticity in the small strain limit, restricted to isotropic damage. Representative models and example problems demonstrate utility and flexibility of this theory for depicting nonlinear hyperelasticity, viscoelasticity, and/or damage from cracks or voids, with physically measurable parameters.

Paul*, S.; and Freed, A. D.: "A simple and practical representation of compatibility condition derived using a QR decomposition of the deformation gradient," *Acta Mechanica,* 231 (2020), 3289–3304. DOI: 10.1007/s00707-020-02702-x

This paper examines a condition for the existence and uniqueness of a finite deformation field whenever a Gram–Schmidt (**QR**) factorization of the deformation gradient **F** is used. First, a compatibility condition is derived, provided that a right Cauchy–Green tensor $\mathbf{C} = \mathbf{F}^{T}\,\mathbf{F}$ is prescribed. It is well-known that under this condition a vanishing of the Riemann curvature tensor **R** ensures compatibility of a finite deformation field. We derive a restriction imposed on Laplace stretch ***U***, arising from a **QR** decomposition of the deformation gradient, through this compatibility condition. The derived condition on Laplace stretch is unambiguous, because a Cholesky factorization of the right Cauchy–Green tensor ensures the existence of a unique Laplace stretch. Although a vanishing of the Riemann curvature tensor provides a necessary and sufficient compatibility condition from a purely geometric point of view, this condition lacks a direct physical interpretation in a sense that one cannot identify the restrictions imposed by this condition on a quantity that can be readily measured from experiments. On the other hand, our compatibility condition restricts dependence of components of a Laplace stretch on certain spatial variables in a reference configuration. Unlike the symmetric right Cauchy–Green stretch tensor **U** obtained from a traditional polar decomposition of **F**, the components of Laplace stretch can be measured from experiments. Thus, this newly derived compatibility condition provides a physical meaning to the somewhat abstract idea of the traditionally used compatibility condition, viz., a vanishing of the Riemann curvature tensor. Couplings between certain components of the Laplace stretch representing shear and elongation play a crucial role in deriving this condition. Finally, implications of this compatibility condition are discussed.

Clayton, J. D.; and Freed, A. D.: "A Constitutive Model for Lung Mechanics and Injury Applicable to Static, Dynamic, and Shock Loading," *Mechanics of Soft Materials*, 2 (2020), 3. DOI: 10.1007/s42558-020-0018-9

A continuum model for lung parenchyma is constructed. The model describes the thermomechanical response over a range of loading rates—from static to dynamic to shock waves—and a range of stress states, including isotropic expansion, triaxial extension, simple shear, and plane wave compression. Nonlinear elasticity, viscoelasticity, and damage are included, with the latter associated with changes of biological function as well

as mechanical stiffness. A Gram–Schmidt decomposition of the deformation gradient leads to strain attributes that enter the thermodynamic potentials as state variables. A free energy function is designed for loading at low to moderate rates and tensile pressures, whereby the tissue response, with surface tension, is preeminent. An internal energy function is designed for wave propagation analysis, including shock waves, whereby compressibility of the air inside the alveoli is addressed via a composite stiffness based on a closed-cell assumption. The model accurately represents the response to triaxial loading, pressure relaxation, and dynamic torsion with relatively few parameters. Longitudinal wave speeds are reasonable for ranges of internal airway pressure and transpulmonary pressure. Airway pressure strongly affects the response to plane wave compression. Criteria for local injury and damage progression depend on a normalized energy density and its gradient, where the latter is paramount for impact problems involving fast pressure rises. Results suggest that local damage associated with edema is induced at load intensities much lower than those that would cause significant stiffness changes due to rupture, major tearing, or local collapse.

Jiang*, M.; Lawson*, Z. T.; Erel*, V.; Pervere*, S.; Nan*, T. Robbins, A. B.; Freed, A. D.; and, Moreno, M. R.: "Clamping soft biologic tissues for uniaxial tensile testing: A brief survey ofbcurrent methods and development of a novel clamping mechanism," *Journal of the Mechanical Behavior of Biomedical Materials*, 103 (2020), 103503.

Biologic tissues are complex materials that come in many forms and perform a variety of functions. They vary widely in composition and mechanical properties, and determination of the mechanical properties of tissues is of interest to those trying to engineer tissues to restore missing function. In performing experiments to characterize the mechanical properties of biologic tissues, there is no single solution to clamping tissues or tissue engineered constructs for mechanical testing. Various clamping techniques have been developed over the past few decades to address the difficulty of imposing appropriate boundary conditions on particular soft tissues during mechanical testing. Two criteria for a successful clamping mechanism are (i) prevention of test specimen slippage, and (ii) prevention of test specimen failure outside the gage region. Herein we present a novel clamping mechanism design developed for the mechanical testing of abdominal wall tissue as an example. This design incorporate pins with serrated clamps to successfully decrease the occurrence of test sample slippage while reducing imposed stress concentrations at the clamping sites. This design was evaluated by performing 40 uniaxial tensile tests on rat abdominal wall muscles using strain rates of 1% per second or 10% per second. Load and displacement data were acquired at the grips. The clamping area on the tissue sample was marked with India ink to track potential slippage of the sample during testing. Ultimate tensile strength and the corresponding stretch were calculated when the maximum load was achieved. With fine-tuning of the torque applied to the clamping grips, the success rate of the tensile tests reached over 90%.

Geotechnical Hazards - Landslides Case Histories

by Pedro Pinto, Member EUAS

Short Biography

● *Licenciated in Civil Engineer (6 years course,1965-1971)(with honors);*
- Industry from 1971 to 1975;
- Master of Engineering 1975 – 1977 (with high honors);
- Specialist in Geotechnique (Ph.D Degree) 1979 - 1983 (with high honors);
- Director of Research (Full Professor degree) (with high honors), since 1992.
● *Related with ISSMGE (International Society for Soil Mechanics and Geotechnical Engineering)*
- Appointed Board member (2017-2021)
- Immediate Past President (2009-2013)
- President (2005-2009),
- Vice President for Europe (2001-2005),
- Chairman of TC4 "Earthquake Geotechnical Engineer Committee" (1994-2000).
● *Full Professor of Geotechnical Engineering of University of Coimbra*
- World Bank Consulting for Dams Safety (2013-2015),
- Invited Professor of Master Courses "Soil Mechanics" and "Engineering Geology" of New University of Lisbon (1983-1995),
- United Nations Consulting for Design and Instrumentation for Dams (1988-1992).
- Invited Guest Lecturer of University of California, USA (1992-1994).
- President of Portuguese Society for Geotechnique (1996- 2000).
● *Pedro Sêco e Pinto is a Consulting Engineer and has participated in more than 450 major projects in Dams, Power plants, Bridges, Tunnels, Landslides and Quay Walls, in Portugal, Angola, Argelie, Brazil, Cabo Verde, China, Dominican Republic, Ecuador, Guine- Bissau, Guine Ecuatorial, India, Lebanon, Malawi, Morocco, Mozambique, Senegal, Syria, Tunisie, Uganda, Venezuela and Zambia, covering field and laboratory testing, dynamic analyses, earthquake engineering, numerical analyses, ground improvement, slopes, special foundations, instrumentation and safety evaluation.*
● *He has presented more than 350 State-of-the Art Lectures and Special Lectures in 80 countries of the 5 Continents.*
● *Pedro Sêco e Pinto has organized, under the umbrella of the International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE), more than 50 International Seminars, since 2006, in Africa (Ghana, Mozambique, Nigeria, South Africa, Sudan), in Asia (Bangladesh, Cambodia, China, India, Indonesia, Kazakhistan, Laos, Malasya, Mynamar, Nepal, Pakistan, South Korya, Sri Lanka, Vietnam), in Australasia (Australia and New Zealand) in Europe (Albania, Belarus, Croatia, Germany, Hungary, Lithuania, Slovenia, Ukranie), North America (Mexico), South America (Argentine, Bolivia, Dominican Republic, Haiti, Ecuador, Panama, Paraguai, Peru, Venezuela).*
● *Pedro Sêco e Pinto has received more than 50 international Awards including American Biographical Institute USA, "Special Volume for the Contributors of Earthquake Engineering, Nagadi Lecture by Indian Geotechnical Society, Széchy Lecture by Hungarian S M Society and Hungarian Academy of Sciences, Nonveiller Lecture by Croatia Geotechnical Society, Sukle Lecture by Slovenia Soil Mechanics Society, Chin Lecture by Huanzhou University (China), Qian Jia Huan Lecture by Hohai University (China) and Chin Fung Kee Memorial Lecture*

by Institute of Engineers of Malasia, 3rd Victor de Mello Lecture by Indian Geotechnical Society and 3rd Braja Das Lecture, GeoMeast 2019, International Congress and Exhibition, Cairo, Egypt.
● Related his role with Editorial Boards and Reviewer he acted as:
- Associate Editor of International Journal of Earthquake Engineering (since 2017)
- Editor in Chief of International Journal of Case Histories (2011-2017)
- Co-Editor of Geotechnical and Geological Engineering Journal, Springer Publisher (2005-2011)
- Member of Editorial Board of several Journals, namely: "Geotecnia", "Bulletin of Earthquake Engineering", "Acta de Geotecnia", "International Journal of Geotechnical Engineering".
- Editor of Proceedings of 4 International Conferences.
● Pedro Sêco e Pinto is author or co-author of 500 Technical and Scientific Reports, more than 180 papers for National and International Conferences and Journals and has contributed for 10 books.

International Activities in 2020

ISSMGE Board Meeting, in Tunis 5th March 2020

International Conference (Tunisie, March, 2020)

Geotechnical Hazards - LANDSLIDES Case Histories (Invited Lecture)

Sêco e Pinto, Pedro Simão
Professor of Geotechnical Engineering, University of Coimbra, Portugal
Specialist Engineer in Geotechnique, National Laboratory of Civil Engineering (LNEC)
President of International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE) (2005-2009)

ABSTRACT

In this paper a introduction to hazards is presented. Two landslides case histories are addressed.
The first case history describes the Castro Daire landslide. The geological and geotechnical characteristics, the excavations issues and the slope stability are presented. The slope failure and the slope stability analysis by different methodologies are discussed.
The second case history deals with the stabilization works of Vila Franca school landslide in Portugal. The lessons arising from technical and non technical factors related with slides are analysed, and the anchored retaining walls to stabilize the slopes are described. The field and laboratory tests are referred, as well as the geological-geotechnical model.
For both case histories the design analyses of slopes and retaining walls were based in Eurocode 7. Some results of the global stability analyses are presented. The seismic design was based in Eurocode 8. The results of anchorages tests to calibrate the design values are presented.

International Conference in Albania, April 2020 (postponed to 2021 due to CV19)

Rehabilitation and Reinforcement of Marina EXPO Breakwaters (Keynote Lecture)

Pedro Simão Sêco e Pinto

Professor of Geotechnical Engineering,
University of Coimbra, Portugal
Specialist Engineer in Geotechnique, National Laboratory of Civil Engineering (LNEC)
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Alexandre Pinto, Professor IST
Rui Tomasio
JETSJ
Lisboa, Portugal

ABSTRACT

The existent Marina breakwaters in Lisbon with 12 m high were designed to sustain the interior variations water level. Due a change of the operation system there was a need to assure the safety conditions of the breakwaters for the variation of both interior and exterior water level. So the need for rehabilitation and reinforcement of the existent breakwaters and the quay wall with 264 m long and 27 m wide became inevitable.
In this paper the design defined by PROMAN office and the alternative design proposed by JETSJ/Somague contractor related the rehabilitation and reinforcement of Marina breakwaters will be addressed.
The geotechnical characteristics of the alluvia material, as well the design parameters, will be described.
The design requirements related the static and seismic analysis of the Marina breakwaters will be presented. Particularly attention and focus of the design of the inclined micropiles with 127 mm of diameter and jet grounting columns with 1.2m of diameter proposed by the Contractor will be given.
The constructions issues defined in the Technical Specifications will be addressed.
The tests performed in micropiles to assess the design assumptions will be described.
The instrumentation plan is referred.

Keywords: Rehabilitation, reinforcement, breakwaters, quay wall, jet-grouting, micropiles

International Conference in Cyprus, September 2020 (postponed to 2021 due to CV19)

Lessons Learned from PREVENTION, MITIGATION AND ANALYSIS OF Landslides - KeyNote Lecture

Pedro Simão Sêco e Pinto
University of Coimbra, Portugal
National Laboratory of Civil Engineering

João Barradas & Arlindo Sousa
National Laboratory of Civil
Engineering (LNEC), Lisboa,Portugal

ABSTRACT

In this paper the triggering mechanics, the prevention and mitigation methods and the risk analysis of landslides are addressed. Two case histories are described. The first case history deals with the stabilization works of a landslide in Santarem, Portugal. The anchored retaining walls founded on micropiles to stabilize the hills are described. The field and laboratory tests are referred, as well as the geological-geotechnical model. The design of the retaining walls was based in Eurocode 7 and in Eurocode 8. The results of anchorages tests and micropiles to calibrate the design values are presented.

The second case history is related with La Josefina site in Ecuador, where a huge failure has occurred with around 30 cubic millions of rock materials killing more than 100 persons. The canyon of the valley was blocked creating a lake with a volume of water higher than 200 cubic millions putting in great risk the cities of Cuenca and Azuogues.

Keyords: landslides, prevention, mitigation, risk analysis, case histories

Advanced Materials for Energy Storage & Conversion

by Zongping Shao, Member EUAS

Short Biography

Zongping Shao, *was born in 1973. He currently is a John Curtin Distinguished Professor at Curtin University, Australia. He obtained his BSc in 1995 from Department of Chemistry, Faculty of Science, Zhejiang University (Xixi Campus, former Hangzhou University) and his Ph.D degree in 2000 from Dalian Institute of Chemical Physics, Chinese Academy of Sciences. After his ph. D graduation, he has been a visiting scholar at Reserches sur la Catalyse, CNRS, France for one and half years (August, 2000-Feburary, 2002), and then a postdoc at Materials Science, California Institute of Technology for three and half years (March, 2002-June, 2005). He joined Nanjing Tech University as a full professor at July, 2005. Currently, he is a John Curtin Distinguished professor at Curtin University. Prof. Shao's major research areas are located at (photo)electrochemical energy storage and conversion and new energy materials, like rechargeable batteries (Lithium-ion batteries, sodium-ion batteries, metal-air batteries, lithium-sulfur batteries, and solid-state batteries), fuel cells, solar cells, and hydrogen production. Up to now, Prof. Shao has published about 550 energy-related papers in various reputed journals, like Nature, Nature Communications, Science Advances, Advanced Energy Materials, Chemical Reviews with a total citation of more than 36,000 and a H-index of 89, one monograph and five book chapters. He was also awarded two US patents and more than 30 Chinese Patents. He has been recognized as one of the highly cited researchers in the section of energy by Elsevier since 2015. He is also selected as world-highly cited researcher by (Thomson Reuters) Clairvate Analytics for the year, 2014, 2017, 2018 and 2019 and 2020.*

Main Research Areas and Publications

Professor Shao's research interests include (1) Mixed conducting membranes for oxygen permeation, (2) solid oxide fuel cells (SOFCs), (3) electrocatalysts for room-temperature oxygen reduction, oxygen evolution and hydrogen evolution reactions (ORR, OER and HER), (4) advanced energy storage devices including lithium/sodium-(ion) batteries, metal-air batteries and supercapacitors, (5) solar cells, etc. He has published more than 650 international journal papers with a total citation of >36000 and an H-index of 89 (Google Scholar). He was selected by Clarivate Analytics as one of the highly cited researchers (2014, 2017-2020). He was also awarded as one of the highly cited Chinese researchers by Elsevier China (2015-2019).

Selected Awards and Honors

1. *Ten-Thousand Talents Program of China, 2019*
2. *Ministry of Science and Technology Innovative Talents Promotion Plan, 2018*
3. *Second Prize in Hubei Province Science and Technology Award, China, 2017*
4. *The Member of EU Academy of Sciences, 2017*
5. *Millions of Talent Projects National Candidates, China, 2017*

6. *Special Government Allowances of the State Council, China, 2016*
7. *Second Prize in Jiangsu Province Science and Technology Award, China, 2015*
8. *Distinguished Award for Novel Materials and their Synthesis by IUPAC& NMS, 2013*
9. *ARC Future Fellowships, 2011*
10. *The Changjiang (Yangtze River) Scholar Award, Chinese Ministry of Education, 2011*
11. *National Science Foundation for Distinguished Young Scholars of China, 2010*
12. *Young Researcher New Star Scientist Award (Scopus), 2010*
13. *"New Century Scientist" Awarded by Chinese Ministry of Education, 2008*
14. *Outstanding Young Scholar Award from Jiangsu Province, China, 2008*
15. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2008*
16. *Fok Ying Tung Research Grant for Excellent Scientist under 35, Education Foundation, Hong Kong, 2007*
17. *One Hundred Most Influential Papers of China, Chinese Institute of Scientific Information, 2007*
18. *First Prize of Advance in Science and Technology of Liaoning Province, China, 2006*

Typical Research

$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), a mixed oxygen-ionic and electronic conductor, was initially developed by Z. P. Shao as a ceramic membrane for oxygen separation from air. In 2004, Z. P. Shao applied BSCF, for the first time, as a cathode material for SOFCs operated below 600 °C. Since then, extensive research has been conducted on intermediate temperature (IT)-SOFCs all over the world. Actually, BSCF has become the hottest cathode material of IT-SOFCs nowadays. This is clearly indicated by the high citations of the paper (***Nature***, 2004, *431*, 170-173; 2332 times as of Jan. 2021). Afterward, Prof. Shao's group continues to develop novel cathode materials for IT-SOFCs, for example, $SrSc_{0.2}Co_{0.8}O_{3-\delta}$ and $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$. The operation temperature of SOFCs was further reduced to the range of 400-600 °C, promoting the development of low-to-intermediate temperature SOFCs.

For protonic ceramic fuel cells (PCFCs), Prof. Shao has developed an oxygen ion/proton/electron conducting nanocomposite, $BaCo_{0.7}(Ce_{0.8}Y_{0.2})_{0.3}O_{3-\delta}$ (BCCY), as a high-performance cathode for PCFCs. Self-assembly during high-temperature calcination results in the formation of a nanocomposite consisting of a mixed H^+/e^- conducting $BaCe_xY_yCo_zO_{3-\delta}$ (P-BCCY) phase, mixed O^{2-}/e^- conducting $BaCo_xCe_yY_zO_{3-\delta}$ (M-BCCY) and $BaCoO_{3-\delta}$ phases. The interplay between these phases promotes the ORR kinetics of this composite cathode and improves its thermo-mechanical compatibility by mitigating the mismatch in thermal expansion coefficient. The ORR activity of this BCCY composite was much higher than most of the reported cathodes for PCFCs, greatly accelerating the commercialization of this technology.

Prof. Shao has also developed perovskite-based anode materials for SOFCs that can

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

For the OER electrocatalysis, Prof. Shao utilized a doping or co-doping strategy to develop several highly active and stable perovskite electrocatalysts (e.g., $SrNb_{0.1}Co_{0.7}Fe_{0.2}O_{3-\delta}$, $BaCo_{0.9-x}Fe_xSn_{0.1}O_{3-\delta}$, and $SrCo_{0.95}P_{0.05}O_{3-\delta}$) and hybrid perovskite-based nanocomposites (e.g., $Ba_{0.35}Sr_{0.65}Co_{0.8}Fe_{0.2}O_{3-\delta}$ with $BaCl_2$ and $SrCl_2$). These catalysts feature well-tailored catalytically active sites and show OER activities that are comparable to or even better than the state-of-the-art precious-metal-based IrO_2. A magnetron sputtering method was further adopted by Prof. Shao to construct amorphous perovskite nanofilms loaded on nickel foam substrate, which gave rise to two orders of magnitude enhancement in OER mass activity. Such amorphous nanofilms can undergo fast reconstruction during electrocatalysis, which was proved to be a universal strategy toward the design of efficient OER catalysts. Prof. Shao found that antiperovskite materials (e.g., $CuNNi_3$) represent another type of active catalysts for the OER. Very recently, through a rational design of silicon-incorporated strontium cobaltite perovskite electrocatalysts, Prof. Shao distinguished the extent of contribution from the participation of lattice oxygen to the OER.

For the HER electrocatalysis, Prof. Shao was the first to demonstrate the capability of perovskite oxides in catalyzing the HER in an alkaline solution. Through a facile A-site praseodymium (Pr) doping into the parent BSCF, he developed $Pr_{0.5}(Ba_{0.5}Sr_{0.5})_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ with well-tuned surface electronic structures and properties, performing competitively with other non-Pt catalysts. Furthermore, novel synthetic methods (e.g., electrospinning, exsolution) were used to develop several nanostructured perovskite-based HER catalysts, which leads to even better catalytic performance. Prof. Shao has developed Ruddlesden-Popper-type Sr_2RuO_4 as a high-performance electrocatalyst for HER in an alkaline solution. It was found out that the improved performance is attributed mainly to the unusual synergistic effect in the layered structure of the Ruddlesden-Popper-type Sr_2RuO_4. Prof. Shao has also developed a single-phase

perovskite $SrTi_{0.7}Ru_{0.3}O_{3-\delta}$ with an unusual super-exchange effect which was beneficial to its highly active and durable HER electrocatalysis in alkaline media.

Derived from his recent intense investigations in room-temperature electrocatalysis, Prof. Shao's also developed highly active bifunctional ORR-OER catalysts (e.g., multicomponent carbon-CoS_x composite, platinum-$Sr(Co_{0.8}Fe_{0.2})_{0.95}P_{0.05}O_{3-\delta}$ perovskite composite) for high-performance and durable zinc-air batteries and developed a unique function-separation electrode design for enhancing both energy density and power density of hybrid zinc batteries.

Career-Best Research Outputs

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A Programmable Polymer Library that enables the Construction of Stimuli-responsive Nanocarriers Containing Logic Gates

by Weihong Tan, Member EUAS

Short Biography

Affiliation: Hunan University，Institute of Basic Medicine and Caner, Chinese Academy of Sciences，Cancer Hospital of the University of Chinese Academy of Sciences

Weihong Tan earned his Ph.D. in physical chemistry at the University of Michigan in 1993. He is the director of the State Key Laboratory of Chemo/Biosensing and Chemometrics and distinguished professor of chemistry and biology at Hunan University. He is also the director of the Institute of Cancer and Basic Medicine, Chinese Academy of Sciences and the dean of the Cancer Hospital of the University of Chinese Academy of Sciences. He served as a University Distinguished Professor and a V.T. and Louis Jackson Professor at the University of Florida for more than 20 years.

Prof. Tan's research is in the general area of bioanalytical chemistry, molecular medicine and chemical biology. He specializes in aptamer research, DNA nanotechnology, and cancer theranostics. He has published over 700 peer-reviewed scientific papers. According to Thomson Reuters, he is among the small, prestigious group of Highly Cited Researchers for the period between 2014-2019. The total citations of his publications exceed 72,000 with an H index of 145. He is currently an associate editor for JACS (Journal of American Chemical Society). He has received over thirty awards and honors, including the Beckman Young Investigator Award in 1997, the Pittcon Achievement Award in 2004, the AAAS Fellow in 2005, the ACS Florida Award in 2012, the Award in Spectrochemical Analysis from the American Chemical Society in 2018, the Prize for Scientific and Technological Progress, Ho Leung Ho Lee Foundation in 2018, the Ralph Adams Award for Bioanalytical chemistry in 2019 and The Pittsburgh Analytical Chemistry Award in 2019. Prof. Tan has also been recognized as an Academician of the Chinese Academy of Sciences in 2015, Academician of the World Academy of Sciences in Developing Countries in 2016, and Member of the European Academy of Science in 2019.

A programmable polymer library that enables the construction of stimuli-responsive nanocarriers containing logic gates

Nature Chemistry

Abstract

Stimuli-responsive biomaterials that contain logic gates hold great potential for detecting and responding to pathological markers as part of clinical therapies. However, a major barrier is the lack of a generalized system that can be used to easily assemble different ligand-responsive units to form programmable nanodevices for advanced biocomputation. Here we develop a programmable polymer library by including responsive units in building blocks with similar structure and reactivity. Using these polymers, we have developed a series of smart nanocarriers with hierarchical structures containing logic gates linked to self-

immolative motifs. Designed with disease biomarkers as inputs, our logic devices showed site-specific release of multiple therapeutics (including kinase inhibitors, drugs and short interfering RNA) in vitro and *in vivo*. We expect that this 'plug and play' platform will be expanded towards smart biomaterial engineering for therapeutic delivery, precision medicine, tissue engineering and stem cell therapy.

DNA-based artificial molecular signaling system that mimics basic elements of reception and response

Nature Communications

Abstract

In order to maintain tissue homeostasis, cells communicate with the outside environment by receiving molecular signals, transmitting them, and responding accordingly with signaling pathways. Thus, one key challenge in engineering molecular signaling systems involves the design and construction of different modules into a rationally integrated system that mimics the cascade of molecular events. Herein, we rationally design a DNA-based artificial molecular signaling system that uses the confined microenvironment of a giant vesicle, derived from a living cell. This system consists of two main components. First, we build an adenosine triphosphate (ATP)-driven DNA nanogatekeeper. Second, we encapsulate a signaling network in the biomimetic vesicle, consisting of distinct modules, able to sequentially initiate a series of downstream reactions playing the roles of reception, transduction and response. Operationally, in the presence of ATP, nanogatekeeper switches from the closed to open state. The open state then triggers the sequential activation of confined downstream signaling modules.

A Cascade Signaling Network between Artificial Cells Switching Activity of Synthetic Transmembrane Channels

Journal of the American Chemical Society

Abstract

Cell–cell communication plays a vital role in biological activities; in particular, membrane–protein interactions are profoundly significant. In order to explore the underlying mechanism of intercellular signaling pathways, a full range of artificial systems have been explored. However, many of them are complicated and uncontrollable. Herein we designed an artificial signal transduction system able to control the influx of environmental ions by triggering the activation of synthetic transmembrane channels immobilized on giant membrane vesicles (GMVs). A membrane protein-like stimulator from one GMV community (GMV_B) stimulates a receptor on another GMV community (GMV_A) to release ssDNA messengers, resulting in the activation of synthetic transmembrane channels to enable the influx of ions. This event, in turn, triggers signal responses encapsulated in the GMV_A

protocell model. By mimicking natural signal transduction pathways, this novel prototype provides a workable tool for investigating cell–cell communication and expands biological signaling systems in general as well as explores useful platforms for addressing scientific problems which involve materials science, chemistry, and medicine.

Transducing Complex Biomolecular Interactions by Temperature-Output Artificial DNA Signaling Networks

Journal of the American Chemical Society

Abstract

The requirement of special expensive instruments for quantitative information readout has significantly restricted sustainable development, from ideation to execution, of advanced artificial networks. Here we present a step toward a paradigm of evolutionary signaling networks that enable translating complex signaling information into easy-to-read temperature output. Combining DNA molecular engineering with basic optical mechanisms, a DNA/Hemin complex-derived versatile temperature-output transducer is established, which can be coupled with other functional modules to fabricate diverse portable DNA signaling networks by dynamic programming of DNA chemical reactions. Its versatility is successfully demonstrated by constructing self-amplified and logic-circuit-based DNA signaling networks to monitor trace and multibit nucleic acid interactions using a thermometer. This affordable yet powerful DNA signaling network design may portend an era of point-of-care signaling network methodology.

Metabolic Labeling of Peptidoglycan with NIR-II Dye Enables In Vivo Imaging of Gut Microbiota

Angewandte Chemie International Edition

Abstract

Deepening our understanding of mammalian gut microbiota has been greatly hampered by the lack of a facile, real-time, and *in vivo* bacterial imaging method. To address this unmet need in microbial visualization, we herein report the development of a second near-infrared (NIR-II)-based method for *in vivo* imaging of gut bacteria. Using $_{D}$-propargylglycine in gavage and then click reaction with an azide-containing NIR-II dye, gut microbiota of a donor mouse was strongly labeled with NIR-II fluorescence on their peptidoglycan. The bacteria could be readily visualized in recipient mouse gut with high spatial resolution and deep tissue penetration under NIR irradiation. The NIR-II-based metabolic labeling strategy reported herein, provides, to the best of our knowledge, the first protocol for facile

in vivo visualization of gut microbiota within deep tissues, and offers an instrumental tool for deciphering the complex biology of these gut "dark matters".

An Aptamer-Nanotrain Assembled from Six-Letter DNA Delivers Doxorubicin Selectively to Liver Cancer Cells

Angewandte Chemie International Edition

Abstract

Expanding the number of nucleotides in DNA increases the information density of functional DNA molecules, creating nanoassemblies that cannot be invaded by natural DNA/RNA in complex biological systems. Here, we show how six-letter GACTZP DNA contributes this property in two parts of a nanoassembly: 1) in an aptamer evolved from a six-letter DNA library to selectively bind liver cancer cells; and 2) in a six-letter self-assembling GACTZP nanotrain that carries the drug doxorubicin. The aptamer-nanotrain assembly, charged with doxorubicin, selectively kills liver cancer cells in culture, as the selectivity of the aptamer binding directs doxorubicin into the aptamer-targeted cells. The assembly does not kill untransformed cells that the aptamer does not bind. This architecture, built with an expanded genetic alphabet, is reminiscent of antibodies conjugated to drugs, which presumably act by this mechanism as well, but with the antibody replaced by an aptamer.

Boron Nitride Nanotube/Nanosheet and In-situ Property Measurement

by Yoshio Bando, Member EUAS

Short Biography

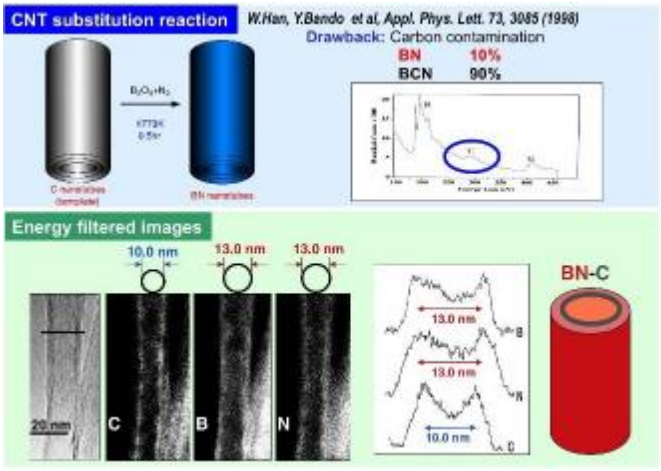
Prof. Yoshio Bando has been leading the communities of nanomaterials and electron microscopy for many years. Holding a PhD degree from Osaka University, he joined the National Institute for Research in Inorganic Materials (NIRIM) in 1975. In 2001, NIRIM was merged with the National Research Institute for Metals to form the National Institute for Materials Science (NIMS), and he was appointed as Director of the Advanced Beam Analysis Group, followed by being appointed Director-General of International Center for Young Scientist. He became a NIMS Fellow in 2004. From 2008 to March 2017, he was responsible for the operation of MANA with the appointed position of Chief Operating Officer (COO). In addition, he was adjunct professor at the University of Tokyo (2009-2012) and guest professor of Waseda University (2008-2016). After retirement of NIMS in 2017, he has been appointed as Distinguished Professor at the University of Wollongong, Australia, and honorary Fellow of NIMS. He is now also Professor at Institute for Molecular Plus, Tianjin University China. He has received many prestigious awards and fellowships, including the "Sacred Treasure" given from the Japanese Emperor in 2017, The 3rd Thomson Reuters Research Front Award in 2012, The Tsukuba Prize in 2005, Academician, The Commendation Award by the Minister of State for Science and Technology in 1998, The Academic Award of the Ceramic Society of Japan in 1997, The Seto Award of Electron Microscopy Society of Japan in 1994 and others. He was appointed as adjunct member of the Science Council of Japan in 2006. He is also a Fellow of the American Ceramic Society and the Royal Society of Chemistry. He served as Editor-in-Chief of Journal of Electron Microscopy and Editorial Board Members of "Nano Energy", "Small", "Nanotechnology", "Materials Horizon", "Nanomaterials" and others. He has been selected as ISI Highly Cited Researcher in Materials Science in 2010, 2012, 2014, 2015, 2016 2017, 2018, 2019, and 2020. To date, he has authored 925 original research papers that have been cited more than 57,219 times with h-index of 125 (Web of Science in December 2020). He has been registered 43 foreign patents and 70 Japanese patents.

Research Activities

Novel synthesis of BN nanotube by a substitution reaction method

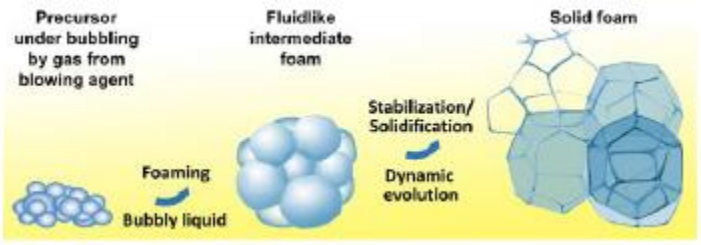
A method involving carbon nanotubes substituted reaction was developed for the synthesis of mass quantities of boron nitride nanotubes. Boron oxide vapor was reacted with nitrogen gas in the presence of carbon nanotubes to form boron nitride nanotubes, whose diameters and lengths are similar to those of the starting carbon nanotubes. It is proposed that carbon atoms of carbon nanotubes can be fully substituted by boron and

nitrogen atoms through a general chemical reaction. The successful preparation of BN-NTs with the average diameters and lengths similar to the starting CNTs confirms the applicability of this method—CNTS substituted reaction. Although the final BN-NTs nanotubes do not contain carbon element, CNTs may play an important role as precursors and in particular supply the skeletons for the growth of BN-NTs during the substitution reaction. After fully substituting the carbon atoms of CNTs by B and N atoms, the B and N atoms of BN-NTs may be involved in a rearrangement process for more suitable and ordered positions at high temperature. Although a deeper understanding of the BN-NTs growth mechanism is clearly needed, we note that this simple and cheap CNTs substituted reaction technology could in principle produce BN-NTs of any quantity. Only sufficient amount of CNT is needed, which have been synthesized in a large quantity and are commercially available. The CNTs substituted reaction developed here is easily accessible to others with an interest in BN-NTs and may also be extended to form nanotubes of other novel materials (for instance, the $B_xN_yC_z$ or C–BN–C sandwich structure nanotubes). The ready availability of large amounts of these nanotubes should offer more opportunities for both new fundamental science and useful nanotechnological applications.



Novel synthesis of BN nanosheet by a chemical blowing method

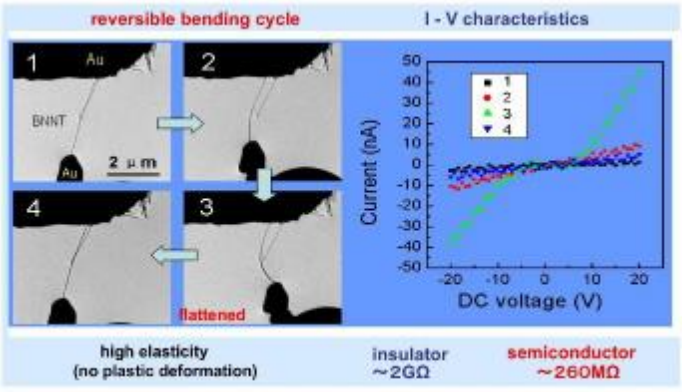
We have developed a new route of chemical blowing for the production of atomically thin (one-to-few atomic layers) free-standing BN and C_x–BN nanosheets. This technology has two main characteristic features: high volume yield and laterally large areas. These not only provide large enough flakes that are readily available for electrical and mechanical performance explorations, but also give enough nanosheet mass for fabricating ultimately strong polymeric or other composites. Significant mechanical reinforcement in PC/BN composites and delicate tuning of nanosheet conductivity through modifying C contents in them are demonstrated in this work. Additionally, this catalyst- and substrate-free method is simpler than a normal CVD method and its products generally possess larger lateral dimensions than those obtained during solution-exfoliation methods. The developed technique opens up a wide horizon for the analogous growth of other 2D nanosheets and full realization of their potentials in nanotechnology.



In-situ mechanical/electrical property measurements of BN nanomaterials under a 300kVTEM-STM/AFM

1. Deformation-driven carrier transport BN nanotube

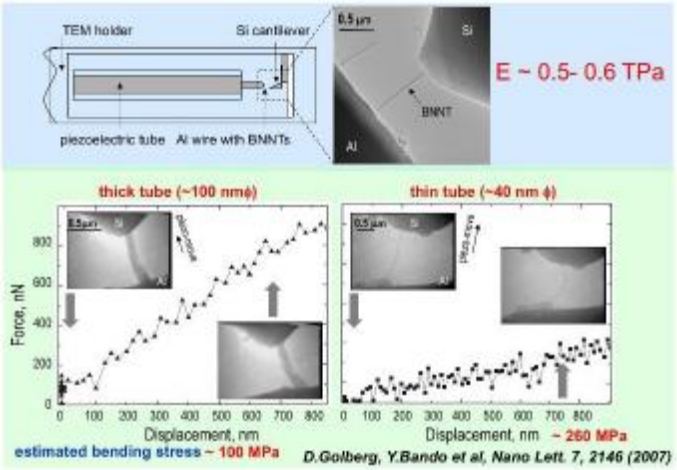
In contrast to standard metallic or semiconducting graphitic carbon nanotubes, for years their structural analogs, boron nitride nanotubes, in which alternating boron and nitrogen atoms substitute for carbon atoms in a graphitic network, have been considered to be truly electrically insulating due to a wide band gap of layered BN. Alternatively, here, we show that under in situ elastic bending deformation at room temperature inside a 300 kV high-resolution transmission electron microscope, a normally electrically insulating multiwalled BN nanotube may surprisingly transform to a semiconductor. The semiconducting parameters of bent multiwalled BN nanotubes squeezed between two approaching gold contacts inside the pole piece of the microscope have been retrieved based on the experimentally recorded I-V curves. In addition, the first experimental signs suggestive of piezoelectric behavior in deformed BN nanotubes have been observed. Remarkably, the nanotube electrical transport properties were found to be smoothly tuned from insulating to semiconducting through a bending deformation. Resultantly, it was confirmed that the unmatched transition in the BNNT electrical performance had been governed by deformation. I-V hysteresis existed in bent BNNTs under the change in a bias voltage sweeping polarity, which could be a sign of BNNT piezoelectricity. Keeping in mind that BNNTs possess excellent mechanical properties and are ultralightweight materials, the discovered deformation-driven tuning of BNNT electrical appearance and piezoelectricity may have many interesting prospective applications in the nanoscale sensors, actuators, and advanced NEMS devices with integrated electronic/optical functions.



X.D.Bai, D.Golberg, Y.Bando et al., Nano Lett. 7, 632 (2007)

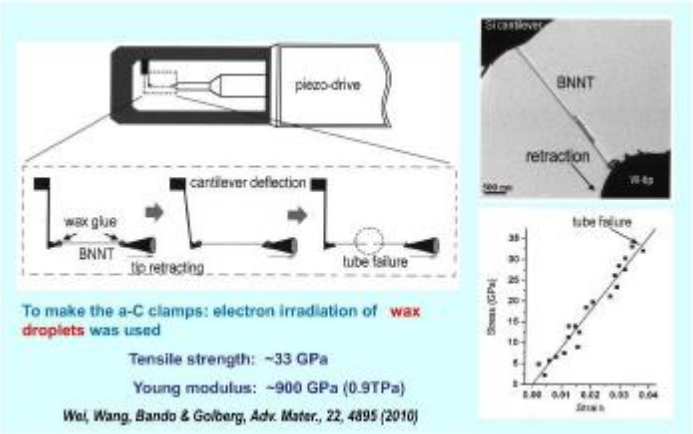
2. Direct force measurement at bending of BN nanotube

Individual multiwalled boron nitride nanotubes of different diameters (40−100 nm) were bent inside a 300 kV high-resolution transmission electron microscope (TEM) using a new fully integrated TEM−atomic force microscope (AFM) piezodriven holder under continuous recording of force−piezodisplacement curves. The tubes were gently compressed in situ (i.e., inside the electron microscope) between a piezomovable aluminum wire and a silicon cantilever. Typically, bending stress values ranging from ∼100 to ∼260 MPa, and corresponding to elastic moduli of 0.5−0.6 TPa, were estimated. Tube gross failures were absent up to very large bending angles (in excess of 115°). Extending the bending angles beyond 30−40° resulted in the elastic deformation of BN nanotubes, which proceeded through the propagation of consecutive momentary kinks. These had the effect of accumulating a bending curvature rather then uniformly curl the tube under the compression load. These kinks were found to be entirely reversible on reloading with no (or marginal) traces of residual plastic deformation.



3. Tensile tests on individual BN nanotube

Tensile loading and pullouts of individual multi-walled BNNTs were studied for the first time by in-situ tests in the integrated HRTEM-AFM setup. Most important mechanical parameters, such as the ultimate tensile strength and strain, maximum sustainable load and the Young's modulus of tubes, were measured. Under parallel HRTEM observations the measured mechanical parameters were correlated to experimental conditions and tube structures. Tensile loading and pullouts of individual multiwalled BNNTs were studied for the fi rst time by in-situ tests in the integrated HRTEM-AFM setup, and the measured mechanical parameters were correlated to experimental conditions and tube structures. All the reported mechanical properties, i.e., continuous shell breakage during pullout, lowering measured breaking strength, unique multishell breakage, are suggested to reflect the partially ionic character of the B-N bonds.



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Control of Complex Granules in Interactive Granular Computing (IGrC)

by Andrzej Skowron, Member EUAS

Short Biography

Andrzej Skowron, *an EurAI (ECCAI) and IRSS Fellow, and the Member of EU Academy of Sciences, received the Ph. D. and D. Sci. (habilitation) from the University of Warsaw in Poland. In 1991 he received the Scientific Title of Professor. He is a Full Professor in the Systems Research Institute, Polish Academy of Sciences as well as in the Digital Research Center of Cardinal Stefan Wyszyński University in Warsaw. He is Emeritus Professor in Faculty of Mathematics, Computer Science and Mechanics at the University of Warsaw. Andrzej Skowron is the (co)author of more than 400 scientific publications and editor of many books and volumes of conference proceedings. His areas of expertise include reasoning with incomplete information, approximate reasoning, soft computing methods and applications, rough sets, rough mereology, granular computing, intelligent systems, knowledge discovery and data mining, decision support systems, adaptive and autonomous systems, perception based computing, and interactive computational systems. He was the supervisor of more than 20 PhD Theses. In the period 1995-2009 he was the Editor-in-Chief of Fundamenta Informaticae, an international journal. He is in the Editorial Boards of many others international journals. Andrzej Skowron was the President of the International Rough Set Society from 1996 to 2000. He has delivered numerous invited talks at international conferences including a plenary talk at the 16th IFIP World Computer Congress (Beijing, 2000), a keynote talk at the 8th Joint Conference on Information Sciences (JCIS 2005) (encompassing 12 individual conferences and workshops) (USA, 2005), an invited talk at the 2006 IEEE/WIC/ACM International Conference on Intelligent Agent Technology (IAT 2006) and on Web Intelligence (WI 2006) (Hong Kong, 2006), and a plenary talk at the 2nd World Congress on Biologically Inspired Computing (Japan,2010). He was serving as (co-)program chair or PC member of more than 200 international conferences. He was involved in numerous research and commercial projects including dialog based search engine (Nutech), fraud detection for Bank of America (Nutech), logistic project for General Motors (Nutech), algorithmic trading (Adgam), control of UAV (Linköping University),and medical decision support (e.g., in Polish-American Pediatric Clinic in Cracow). Andrzej Skowron was in the ICI Thomson Reuters/ Clarivate Analytics lists of the most cited researchers in Computer Science (globally) in 2012, 2016, 2017.*

This article is a continuation of the article *Toward Data Science Computing Model: Interactive Granular Computing* (IGrC) by Andrzej Skowron published in EU ACADEMY 2019 ANNUAL REPORT and is focused about the control of complex granules. More details about IGrC can be found on this site https://dblp.org/pid/s/AndrzejSkowron.html in papers related to IGrC**.** The control

of c-granules will be discussed in more detail in the keynote by Andrzej Skowron at the *Fourth International Conference on Intelligence Science* (ICIS2020) (https://www.icis2020 nitdgp.com) and in the paper (co-authored by Dr. Soma Dutta) in the Proceedings of ICIS2020.

Abstract

The problem of understanding intelligence is treated, by some prominent researchers, as the greatest problem of this century. In the recent issue of ERCIM, entitled as *Smart Things Everywhere*, there is an explanation of the title; it emphasizes that the title refers to more than that of Internet of Things or Industrial Internet of Things as it encompasses, in particular, intelligence, cognitive systems and technology, machine learning and AI. In this article we claim that to justify a decision support systems to be intelligent there is a need for developing new reasoning tools which can also take into account the significance of the processes of sensory measurement, experience and perception about the concerned situations in the physical world; i.e., understanding (to a satisfactory degree) the process of obtaining information about a situation, in the physical world, is also required for making relevant decisions. The reasoning, called (adaptive) judgment, is performed over objects interacting in the physical world using Interactive Granular Computing Model (IGrC). The basic objects in IGrC are called the *complex granules* (*c-granules*, for short). The c-granules, which are extended by information layers, are called *informational c-granules* (*ic-granules*, for short), and they can create the basis for modeling a notion of control conducting the whole process of computation realized by the c-granule. Through the ic-granules the control of a c-granule can link the abstract and physical worlds, and help to realize the paths of judgments starting from sensory measurement, experience to perception.

1. Motivation

In the book by Gerrish entitled *How Smart Machines Think* (Press, Cambridge, MA 2018), ideas related to thinking by a smart machine are discussed, and in particular, perception and interaction with the world are pointed out:

I'll outline some of the key ideas that enable intelligent machines to perceive and interact with the world.

Existing approaches to soft computing, such as rough sets, fuzzy sets, and other tools used in machine learning lack in considering the above mentioned two components. There are two prevalent traditions of mathematical modeling. One is *purely mathematical* where it is considered that the sets are given. For example, in the case of the rough set approach, the starting point is the universe of objects and an indiscernibility or similarity relation(s); further developments on approximating concepts are made on this basis. In the context of fuzzy sets, the universe of objects and some basic fuzzy membership functions, relative to some concepts, are assumed as given; based on that fuzzy membership functions for other complex concepts are induced. The second tradition of modeling may be called *constructive*, where it is assumed that objects are partially perceived by means of some features or attributes, and only a partial information about these objects in the form of vectors of attribute values is available. On this basis indiscernibility or similarity relations are defined and

further developments are carried out (assuming often that information about sets of objects is also partial). This approach is often followed in rough sets. In the context of fuzzy sets also often this approach is used, i.e., the fuzzy membership functions are constructed based on a set of attributes and then they are ascribed over the universe of objects. Both the traditional modeling do not take into account *how* the process of perceiving attribute values is realised, *where* and *how* to access the concerned objects in the physical space, and *why* those attributes are selected. Hence, clearly the perception and action are out of the scope of such practices of modeling. However, this is crucial for many tasks, especially, when we are dealing with complex phenomena in the real physical world. As a result, characterization of the state of the complex physical phenomena by a fixed set, or a priori set of attributes becomes irrelevant. From a similar concern, the researchers (see AI Magazine 37, 2016) proposed to extend Turing test by embedding into it the challenges related to action and perception.

So, how a function representing a particular vague concept is learned from the uses of the community, as well as which parameters to be considered crucial in (approximate) defining a vague concept and how the values for these parameters are observed or measured, incorporating such information in the model is important for an intelligent agent; otherwise a non-human system cannot derive the relevant information about unseen so far cases. Hence, we need an extension of the existing approaches where apart from the information about a physical object, a specification of how the information label of a physical object is physically linked to the actual object also can be incorporated.

The readers are referred to the article *Toward Data Science Computing Model: Interactive Granular Computing* (IGrC) by Andrzej Skowron published in *EU ACADEMY 2019 ANNUAL REPORT* for more comments related to motivation of the discussed approach.

2. From complex granules (c-granules) and informational complex granules (ic-granules) to control of c-granules

In IGrC it was recognised (see papers on interactive computations on https://dblp.uni-trier.de/pers/hd/s/Skowron:Andrzej) the necessity of introducing *complex granules* (*c-granules*, for short). The computations in the IGrC model are realized on the interactive complex granules and the progress of the computation process is based on the consequences of the interactions occurring in the physical world. Hence, the computational models in IGrC can't be constructed solely in an abstract mathematical space. The proposed model of computation based on complex granules seems to be of fundamental importance for developing intelligent systems dealing with complex phenomena, in particular in such areas as Data Science, Internet of Things, Wisdom Web of Things, Cyber Physical Systems, Complex Adaptive Systems, Natural Computing, Software Engineering, and applications based on Blockchain Technology, etc .

In the discussed approach, we assume that physical objects exist in the physical space and are embedded into its parts. Physical objects are interacting in the physical space, and thus some collections of physical objects may create dynamical systems in the physical space. It is important to explain how properties of these objects and interactions among them can be perceived by c-granules. In our attempt, to design c-

granules with the ability of perceiving physical objects and their interactions, this is realised by the control mechanism of c-granule based on *informational complex granules* (*ic-granules*) and a special kind of reasoning over them, called judgment. Following Heller (see H. Heller, M.: *The Ontology of Physical Objects. Four dimensional hunks of matter*. Cambridge Studies in Philosophy, Cambridge University Press, Cambridge, UK, 1990), it is worthwhile to refer to the concept of physical objects as four-dimensional hunks of matter. However, in our approach, four-dimensional hunks of matter are relative to a given c-granule and are localised by means of formal spatio-temporal windows specified in the informational layer of the c-granule; this corresponds to the parts of the physical space in which hunks of matter are embedded.

Informational complex granules (ic-granules) are constructed over two basic ingredients: abstract and physical; we may count these two ingredients respectively as informational and physical objects. Abstract ingredients of ic-granules consists of families of formal specifications of spatio-temporal windows labelled by information, expressed in a formal or natural language, specific for a given c-granule or a family of c-granules. The information may be of different kinds and may have different forms. Moreover, one of the ic-granules encodes in its information layer the local (discrete) time clock and enables the model to perceive features of physical objects at different moments of time and to reason about their changes. For example, the information layer of an ic-granule may contain formulas and their (expected or real) degrees of satisfiability at a given moment of time on some physical objects, as well as the formal specifications of the spatio-temporal windows indicating the location and (perception) time of those physical objects. It can be a Boolean formula over atomic formulas of the form $a =_t v$ specifying the value of attribute *a* is *v* at a given moment of time *t*, or can be a more compound expression, encoded in an information system containing results of measurements in time for vectors of attributes of the objects related to the given (in informational layer) formal specifications of spatio-temporal windows.

The physical layer of any ic-granule is called c-granule and is divided into three parts: *soft_suit, link_suit* and *hard_suit*. Each of these parts is a collection of physical objects. The *hard_suit* consist of the physical objects that are to be perceived. The *soft_sui*t is considered to have those objects which are *directly accessible* at a particular point of time. The objects in the *link_suit* allow us to create, in a sense, a *physical pointer* that links objects from the *soft_suit* to the *hard_suit*; this in turn makes it possible to propagate interactions among physical objects, in particular among objects of *hard_suit* and *soft_suit*. By directly accessible we mean that some features (or attribute values) of such objects can be directly measurable, or changes of some features (or attribute values) of such objects in successive moments of local time of the c-granule (or in a given period of time) can be directly measurable, or some features (or attribute values) of such objects can be directly changed by a mechanism like control. It should be noted that some features of not directly accessible objects can be derived by control using judgment over the already perceived features with a support of knowledge bases or physical laws represented in some ic-granules.

The behavior of the control of a given c-granule can be divided into cycles. Each cycle of the control of a given c-granule starts from a current configuration (family) of ic-granules. This configuration contains a distinguished ic-granule with information representing the perception status of the current situation. Each cycle consists of

several steps such as modification, deletion, suspension of ic-granules or generation of some new ic-granules from the current configuration. It should be noted that a special kind of ic-granule, called *implementation ic-granule, is* used for generation of new ic-granules from their formal specifications. Once a new configuration of ic-granules is created the control measures features of some new physical objects in the scope of the newly developed ic-granules and/or matches or aggregates information with that of the previous ic-granules using its judgment mechanism. The cycle ends when the control gathers perception, to a satisfactory degree, about the current configuration, and becomes able to take a relevant decision with respect to the goal of the computation process.

Formal specification of many complex tasks or formal specification of c-granule needs may be thought of as a *complex game* consisting of a family of complex vague concepts, labeled by actions or plans (represented by the relevant formal specification ic-granules) that to be performed when the concepts are satisfied to a satisfactory degree. These complex vague concepts may describe, e.g., invariants which should be preserved to a satisfactory degree, conditions representing degrees of risk of disaster in the environment perceived by the system, safety properties of trajectory of granular computations, conditions representing the quality of the current path from the point of view of carried out computation toward the target goals, or risk concerning a possibility that the current needs are no longer achievable. It should be noted that these complex vague concepts (usually described in a fragment of a natural language) should be learned from data and domain knowledge with the use of physical laws. During perception of the current situation in the physical world the control uses its judgment tools over information gathered from information layers of dynamically changing (by control and the environment) configurations of the ic-granules. Moreover, the concepts as well as their labels, involved in a complex game, are evolving in time. Hence, the control should have some adaptive strategies allowing relevant modification of the complex game.

We would like to emphasize the role of reasoning, called judgment, for the control of a c-granule. The further development of judgment methods will play the principal role in further development of intelligent systems. These reasoning methods are far beyond the existing deductive methods so well already developed in mathematical logic or even inductive reasoning (e.g., in Machine Learning). They should take into account, e.g., experience as well as explanation of behaviour. These reasoning methods should be grounded on a new computing model making it possible to perform reasoning from sensory measurement to perception (i.e., understanding the perceived situation). We propose to base such a model on interactive complex granules (c-granules) having their informational parts grounded in the physical world.

Laser Precision Manufacturing and Microsphere Lens Nano-Imaging

by Lin Li, Member EUAS

Short Biography

Professor Li obtained a BSc degree in Control Engineering from Dalian University of Technology (China) in 1982 and a PhD degree in Laser Engineering from Imperial College London in 1989. He worked at University Liverpool (UK) between 1988-1994 as a Research Associate and Research Fellow in laser materials processing and became a Lecturer in manufacturing at UMIST (University of Manchester Institute of Science and Technology), UK and promoted to a full Professor in Laser Engineering and Director of Laser Processing Research Centre in 2000. He served as head of manufacturing research group 2004-2014, Deputy Head of School (Research) of School of Mechanical, Aerospace and Civil Engineering 2009 -2013, and Associate Dean (Business Engagement and Innovation) 2015-2020 at The University of Manchester, UK.

Professor Lin Li is an elected fellow of Royal Academy of Engineering (UK), fellow of International Academy of Production Engineering, fellow of International Academy of Photonics and Laser Engineering, fellow of Laser Institute of America, and fellow of Institute of Engineering and Technology.

He has served as the President of Laser Institute of America (2016), President of International Academy of Photonics and Laser Engineering (2013-2015), and President of Association of Industrial Laser Users (AILU – 2017-2019).

Professor Li is the author and co-author of over 600 scientific publications of which over 400 are in peer-reviewed journals related to the science, technology and applications of laser based manufacturing and photonics. Professor Li is an inventor of the microsphere lens super-resolution optical microscope that has broken the optical diffraction limit. The technology has been commercialized and super-resolution microsphere lens (SMAL) based optical nanoscope has been sold worldwide. He is a pioneer of industrial laser cleaning of metallic alloys that have been successfully used in the aerospace and automotive industries for welding preparations. He is also an inventor of laser powder bed fusion based multiple material additive manufacturing (3D printing) technology.

He received Arthur Charles Main Award from the Institute of Mechanical Engineers in 2001 for work in laser based nuclear decommissioning technology. He received the Sir Frank Whittle Medal from the Royal Academy of Engineering (UK) in 2013 for innovative manufacturing that has led to economic impacts. In 2014 he received Wolfson Research Merit Award from the Royal Society for his research on laser nano-fabrication and nano-imaging, and received Researcher of the Year medal from The University of Manchester in 2014. In 2019 he received Arthur Schawlow medal from Laser Institute of America for his contribution to advancing laser processing science and technology. He received Donald Julius Groen Prize from Institution of Mechanical Engineers in 2019 for his leadership in advancing additive manufacturing science, technology and education.

Selected Publications

1. ***Z.B.Wang, W.Guo, L.Li, B.Luk'yanchuk, A,Khan, Z.Liu, Z.Chen and M.H.Hong, "Optical virtual imaging at 50 nm lateral resolution with a white-light nanoscope", Nature Communications, Vol. 2, Issue 218, 2011, DOI:10.1038/ncomms1211***

   Optical microscope is inherently limited in resolution by optical diffraction limit to half of the optical wavelength. For visible light of 400-700 nm wavelengths, this theoretical imaging resolution is 200 nm. This research demonstrated a new imaging method utilising transparent microsphere lenses placed in the virtual imaging plane of standard optical microscope allowing the direct optical imaging resolution to reach 50 nm. This work has led to a new field of study in optics and commercialisation for optical nanoscopy.

2. ***L.Li, W.Guo, Y.Z.Yan, S.J.Lee, T.Wang, "Label-free super-resolution imaging of adenovirus by submerged microsphere optical nanoscopy" Light: Science and Applications, Vol. 2, 2013, E60, doi:10.1038/lsa.2013.60***

   Most viruses have sizes below the standard optical microscope imaging resolution limit of 200 nm. This research demonstrated a method of optical imaging using submerged microsphere lens to allow the direct observation of denovirus of 75 nm in size, breaking the theoretical optical diffraction limit of optical microscopes. The associated scientific mechanism is described. This technology has been commercialized.

3. ***Y.Z.Yan, L.Li, C.Feng, W.Guo, S.Lee, M.H.Hong, "Microsphere-coupled scanning laser confocal nanoscope for sub-diffraction-limited imaging at 25 nm lateral resolution in the visible spectrum", ACS Nano, Vol .8 Issue 2, 2014. pp.1809-1816. DOI: 10.1021/nn406201q.***

   By combining microsphere lenses with a confocal microscope, direct optical imaging resolution has been demonstrated to reach 25 nm well beyond the theoretical optical diffraction limit of 200 nm for visible light. The fundamental scientific principles were proposed.

4. ***C.Wei, L.Li, X.J.Zhang, Y.H.Chueh, "3D printing of multiple metallic materials via modified selective laser melting" CIRP Annals-Manufacturing Technology, Vol. 67, Issue 1, 2018, pp. 245-248, DOI: 10.1016/j.cirp.2018.04.096***

   Additive manufacturing is an emerging manufacturing technology that

components of complex geometry to be manufactured without the need for a die or mould. Additive manufacturing of metallic materials is currently limited to single material. It is desirable to be able to tailor material properties at different locations of a component. This research set a new milestone in additive manufacturing to show that multiple metallic material additive manufacturing is possible with combined powder-bed fusion and point-by-point ultrasonic powder deposition and powder removal.

5. ***Y.Huang, L.Zeng, C. Liu, D.Zeng, Z.Liu, X. Liu, X.Zhong, W.Guo and L.Li, "Laser direct writing of heteroatom (N&S) doped graphene from a polybenzimidazole (PBI) ink donor on polyethylene terephthalate (PET) polymer and glass substrates", SMALL, Vol. 14, issue 44, Nov. 2018. Article number: 1803143.***

   Graphene is a 2D material that has superior electrical and thermal conductivities. Deposition of patterned graphene on a substrate is desirable for a wide range of applications including sensors and batteries. This research demonstrates a new method of depositing patterned and doped graphene by a laser photo-chemical process changing an organic ink into graphene on a substrate. This also allows the tuning the energy gap of graphene.

Concrete Pavement Performance, Rehabilitation, Behavior & Design

by Dan G. Zollinger, Member EUAS

Short Biography

Professor
Civil Engineering
Texas A&M University

Professional Interests

Pavement Design, Behavior, and Performance
Mechanical and Material Properties of Concrete
Non-Destructive Testing of Pavements
Fracture and Damage Mechanics
Concrete Mixture Design and Concrete Paving

Research Engineer
Texas Transportation Institute
Texas A&M University

Education

B.S., Civil Engineering, Utah State University, 1977
M.S., Civil Engineering, Utah State University, 1981
Ph.D., Civil Engineering, University of Illinois, 1989

Experience

Professor, Civil Engineering, Texas A&M University, College Station, Texas, September 1, 2006 to Present.
Associate Professor, Civil Engineering, Texas A&M University, College Station, Texas, September 1, 1994 to September 1, 2006.
Assistant Professor, Civil Engineering, Texas A&M University, College Station, Texas, November 1, 1988 to August 31, 1994.
Consulting Airport Engineer, Reinard W. Brandley, Sacramento, California, July 1981 - August 1984.
Airport Design Engineer, Salt Lake City International Airport, Salt Lake City, Utah, April 1980 - June 1981.
Geotechnical Engineer, Dames & Moore, Salt Lake City, Utah, September 1979 - April 1980.

Professional Licenses

Registered Professional Engineer: California #35726, Texas #67129, Oklahoma # 29676

Dr. Dan G. Zollinger is a Professor at Texas A&M University in the Department of Civil Engineering and a Research Engineer at the Texas A&M Transportation Institute (TTI). He is the former manager for the rigid pavements program at TTI and is a Past President and an Honorary Member of the International Society for Concrete Pavements (ISCP). He is very knowledgeable of construction methods and procedures for concrete pavement systems and their effect on pavement performance. His major areas of research include concrete pavement performance, rehabilitation, behavior, and design. He was a consultant on the development of the 200x AASHTO Guide (NCHRP Project 1-37a) and played a key role in the advancement of the design of CRC pavements. He is actively engaged in pavement evaluation, pavement design, and pavement performance particularly as it may be affected by the joint seals. His has worked for several years on the development of performance models for mechanistic pavement design procedures; this effort has led him to collect performance data from a variety of concrete pavement sections to

validate an array of distress mechanisms for concrete pavement ranging from punch out distress to faulting. He has also researched for several years the structural behavior of concrete materials under field conditions and the evaluation of drainage related performance as a function of base type, drainage effectiveness, erosion resistance, and joint sealant performance. This effort has also led to the formulation of erosion damage model account as a function of abrasion wear on the surface of the base layer, the bulk plasticity particularly of unbound base layers, and the moisture impermeability of the joint sealant system and its effect on the number of wets days associated with the moisture in the joint cavity. He has recently been involved in the development of a new test method for erosion in concrete pavements. He has been involved with several projects dealing with pavement instrumentation and testing and serves on several technical committees related to the behavior of rigid pavements. More recently, he has been researching the performance of RCC pavement in Texas doing several FWD collection and instrumentation of RCC construction. .

His major areas of research include concrete pavement materials, performance, behavior, design and repair. He has also researched for several years the curing and setting behavior of concrete materials under both lab and field conditions and the effect of curing on performance as a function of material combinations, mixture characteristics, and method of construction. He has been engaged in pavement instrumentation and pavement testing studies focusing on the control of early age pavement cracking, and other studies regarding the effect of aggregate size and shape distribution characteristics on the placeability and workability of the paving concrete.

Dr. Zollinger has had extensive experience in the area of pavement evaluation and the subsequent development of performance prediction models for concrete pavements based on the measured and back-calculated properties and database performance characteristics. He has just recently been involved with one national research project focusing on the development of guidelines for the rehabilitation of the concrete pavements and another one focusing on pavement evaluation relative to the appropriate selection of rehabilitation treatments. He was worked several years as a resident engineer for the SLC International Airport and a design engineer for Reinard W. Brandley, consulting airport engineer in Sacramento, California.

He also led an effort to develop a survey guide to identify ASR in airfield pavement structures on the behalf of the Federal Aviation Administration (FAA). The development process involved the formulation of a simple format to assist airfield maintenance and repair personnel in decisions regarding the rehabilitation of the airfield pavements damaged by ASR. Identification of ASR based on visual inspection is very complicated and requires clear and logical thinking to formulate a simple and non-complex solution to help practicing engineers understand ASR distress and the extent of its severity. The development of the methodology was orchestrated to fit in with the present PCI method of pavement survey rating and accounted for critical indicators of possible ASR such as key combinations of visual distress types, climatic conditions, and material combinations. These factors were used to formulate a rating scheme, which indicates the degree of ASR distress severity.

Selected Refereed Journal Publications

Zollinger, Dan G. and Ernest J. Barenberg, "Field Investigation of Punchout Distress in CRC Pavement in Illinois," Transportation Research Record, *Highway and Facility Design*, No. 1286, pp. 1-13, TRB, Washington, D.C., 1990.

Tang, Tianxi, Dan G. Zollinger, and Sanjaya P. Senadheera, "Analysis of Concave Curling in Concrete Slabs," Vol. 119 No. 4, ASCE Journal of Transportation Engineering, July/Aug 1993, pp. 618-633.

Senadheera, Sanjaya P., Dan G. Zollinger, "A Framework for Incorporation of Spalling in the Design of Concrete Pavements," Transportation Research Record, *Design and Rehabilitation of Pavements*, No. 1449, pp. 114-122, Washington D.C., 1994.

Tayabji, Shiraz D., Peter J. Stephanos, and Dan G. Zollinger, "Nationwide Field Investigation of Continuously Reinforced Concrete Pavements," Transportation Research Record, *Pavement Design and Analysis*, No. 1482, pp. 7-18, Washington D.C., 1995.

Gurjar, Ashok, Tianxi Tang, and Dan G. Zollinger, "Laboratory Study of Strain and Age Effects on a Concrete Pavement Joint Sealant," Transportation Research Record, *Work Zone Safety and Pavement Markings and Materials*, No. 1529, Washington, D.C., 1996, p. 95-100.

Jeong, Jin-Hoon and Dan G. Zollinger, "Characterization of Stiffness Factors Relative to the Design of Continuously Reinforced and Jointed Pavement," Transportation Research Record, Journal of the Transportation Research Board, No. 1778, Washington, D.C., 2001, p. 54-63.

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Jeong, J. H*. and Zollinger, D. G., "Development of Test Methodology and Model for Evaluation of Curing Effectiveness in Concrete Pavement Construction," *Transportation Research Record*: *Journal of the Transportation Research Board 1861*, pp. 17 – 28, 2003.

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Liangliang Chen; Dan Zollinger, Ph.D.; Bo Tian, "An Approach to Local Calibration of an Advanced Model for Punchout Distress Using LTPP Data," Ref: Ms. No. TEENG-2644R1, Accepted for publication in ASCE's Journal of Transportation Engineering, Feb 2015.

Bakhsh, K. and Zollinger, D., "Faulting Prediction Model for Design of Concrete Pavement Structures," Geo-Shanghai 2014, ASCE *Pavement Materials, Structures, and Performance*, pp. 327-342, http://dx.doi.org/10.1061/9780784413418.003

Sun, Peizhi and Dan G. Zollinger, "Concepts to Enhance Specification and Inspection of Curing Effectiveness in Concrete Pavement Design and Construction," *Journal of the Transportation Research Board (2504)*, 2015, pp. 124-132, http://dx.doi.org/10.3141/2504-15

Mirsayar, M.*, Kaijian Huang, and Dan G. Zollinger, 'A New Approach to Concrete Slab Lift-Off Using Interfacial Fracture Mechanics Concepts," Transportation Research Record, *Journal of the Transportation Research Board (2590)*, 2016 pp 10 -17, http://dx.doi.org/10.3141/2590-02

Neshvandian, K, M. Tyler Speakmon*, and Dan G. Zollinger, 'An Approach to Infiltration Modeling for Partially-Sealed Joints in Concrete Pavement Design," Journal of Materials in Civil Engineering, Vol. 29, Iss. 9, pg 04017121, 2017, https://doi.org/10.1061/(ASCE)MT.1943-5533.0001856.

X Luo, F Gu, Y Zhang, RL Lytton, D Zollinger, "*Mechanistic-empirical models for better consideration of subgrade and unbound layers influence on pavement performance*," *Transportation Geotechnics*, Elsevier, Vol. 13, pg 52-68, 2017, https://doi.org/10.1016/j.trgeo.2017.06.002.

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Pavement Containing Reclaimed Asphalt Pavement Using Pavement ME Models," International Journal of Pavement Engineering, DOI: 10.1080/10298436.2018.1533134.

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Recent Contributions in Materials Science and Engineering

by Derek O. Northwood, Member EUAS

Short Biography

Professor Derek O. Northwood is a Distinguished University Professor and Professor of Engineering Materials in the Department of Mechanical, Automotive and Materials Engineering at the University of Windsor, Windsor, Ontario, Canada. Professor Northwood has an earned doctorate in Chemical Physics (Crystallography) from the University of Surrey (UK) and a BSc (Eng) in Engineering Metallurgy from the Imperial College, University of London (UK). He is a licensed Professional Engineer in Ontario, Canada (PEng) and is a Chartered Professional Engineer (CPEng; NER), APEC Engineer, and International Professional Engineer (IntPE(AUS), in Australia. In the 40+ years as an academic, Professor Northwood has held various administrative positions including Department Head, Dean, Associate Dean of Research, Director of the Office of Research Services, President of the Industrial Research Institute, and, Research Leadership Chair, both at the University of Windsor and Ryerson University, Toronto, Canada. Professor Northwood has taught, researched and facilitated joint research and educational programs at 14 universities worldwide, including the UK, the USA, Australia, Taiwan, China, Singapore and Canada. He has published 687 papers in refereed international journals and conference proceedings, 9 chapters in books and has edited 7 books, on a wide range of topics including materials and their applications, and engineering and technology education. He has been elected Fellow of five international professional societies in Australia, Canada, the UK and the USA; namely, Fellow of the Royal Society of Canada (FRSC); Fellow of the Institution of Engineers Australia (FIEAust); Fellow of the World Institute for Engineering and Technology Education (FWIETE); Fellow of the Institute of Materials, Minerals and Mining (FIMMM); and Fellow of ASM International (FASM). On October 1, 2019 in Portland, Oregon, USA, Professor Derek O. Northwood was inducted as a Fellow of Alpha Sigma Mu (FAΣM), The International Professional Honor Society for Materials Science and Engineering.

Professor Northwood was recently recognized as being among the world's top 100,000 - or top 2% of scientists - according to the database published by Stanford University. The database recognizes the long-term career performance of scientists around the world, living or deceased, who are the most cited authors in their disciplines. It reflects six citation metrics, including total citations and number of citations to papers as single or first author between 1965 and 2019. The data was collected from the Scopus database of nearly 7 million authors out of which the top 100,000/2% were analysed.

RESEARCH ACTIVITIES AND PUBLICATIONS 2020

Covid-19 restrictions have had a negative impact on our ability to conduct research both in my home university and with my partners across the globe.

In my 2019 Annual Report, I reported on the initiation of a research program on the electrospinning of polymer nanofibres. The polymer chosen was polyethylene oxide (PEO) which is a highly crystalline polymer that is non-toxic, biocompatible, biodegradable and can be produced as porous fibres. Nanofibres are used in a wide range of applications including: biomaterials; cosmetic skin masks; nano sensors; military protective clothing; electronic materials. PEO, in the form of a nanofibrous membraned, is

showing considerable promise as a solid polymer electrolyte (SPE) in lightweight lithium secondary batteries.

During 2020, M.A.Sc. (Master of Applied Science) student, Ms. Nehal Faldu, completed her studies on the effect of the molecular weight of PEO on the shape, size, and morphology of the fibres produced by electrospinning. Molecular weights from 100,000 to 5,000,000 g/mol were investigated. The results of this study can be found in Ms. Faldu's M.A.Sc. Thesis, "Electrospinning of PEO Nanofibers, University of Windsor, December 2020

ABSTRACT: Electrospinning is a method centered on electrostatic forces for fabricating continuous nanofibers with a substantial active surface area per mass unit. One of the essential parameters that affect a polymer's ability to create nanofibers is the chain length, given by the molecular weight. In this study, polyethylene oxide (PEO) with molecular weights from 100,000 to 5,000,000 Da were used to investigate the effect of molecular weight on the shape, size, and morphology of the fabricated fibers. The electrospinning experiments were conducted at flow rates ranging from 4.16 to 16.67μL/min and working distances between 10 and 20 cm. The collected fibers were analyzed using Scanning Electron Microscopy (SEM). Based on the solution and processing conditions, different structures from droplets, and heavily beaded fibers to defect-free mats were obtained. PEO's water-based solutions produced bead free fibers for molecular weights in the range of 100,000 to 900,000 Da for a range of processing conditions. However, the processing window for the formation of bead free fibers was more restricted for water-ethanol solutions than for deionized water solutions. Furthermore, the electrospun jet of ultra-high molecular weight PEO (5,000,000 Da) solutions showed very small bending instabilities, which reduced the chance of drying the jet during its flight time, even with a relatively high working distance (20cm). Therefore, the products exhibited over-wetting and film formation. The results are discussed in terms of the viscosity and entanglement number, (ηe) soln, of the PEO solution.

This study was done in conjunction with Associate Professor Reza Riahi and Mr. Iman A. Borojeni at the University of Windsor. A joint paper on the work was to be presented, but the planned conference was postponed until 2021.

Northwood, D.O., Faldu, N., Borojeni, I.A., Riahi, R., "Electrospinning of Polymeric Nanofibres : Effect of Material and Processing Parameters", Plenary Address (Abstract Only), International Conference on Nano Research and Development (ICNRD-2020), Singapore, March 12-14, 2020. *Due to COVID-19, conference is tentatively rescheduled to March 2021.

Research activities have also continued in two other areas.

1. Developing the potential properties of traditional materials.

2. Innovation in Engineering Education.

1. Developing the potential properties of traditional materials

This is part of my ongoing collaboration with Professor Cheng Liu, College of

Mechanical Engineering, Yangzhou University, Jangzhou, China which has resulted in 28 publications on steels, cast irons, aluminum alloys and zirconia ceramics. Research in 2020 was concentrated in two areas, namely high nitrogen austenitic stainless steels, (HNSS) and the development of a heat treatment for enhancing the properties of disc springs made from 60Si2Mn steel. HNSS are important because of their excellent corrosion resistance and good mechanical properties. Work in 2020 focussed on understanding the generation and microstructural characteristics of the surface layer formed during solution treatment of a HNSS. By using a multi-step austempering nanoprocess, a multi-phase nanostructured microstructure is formed in the spring steel which allows for applications involving higher loading and fatigue conditions. Example publications include:

Li, J., Hang,Y., Zhou, S., Wang,X., Liang, Z., Zhou, W., Northwood, D.O., Liu, C.

Multi-phase nanostructured 60Si2Mn disc spring by a novel austempering process
(2020) WIT Transactions on The Built Environment. 196, pp. 11-18

Abstract
A disc spring, also known as a Belleville spring, is a conical shell which can be loaded along its axis either statically or dynamically. It can generate a high force in a very short spring length with minimal movement when compressed. A novel multi-step austempering heat treatment process is developed to improve both the hardness and strength of a conventional 60Si2Mn disc spring. In this case, the disc spring is austenitized at 900°C for 0.5 h, control-quenched to a temperature below Ms (the starting temperature of martensite transformation) for a very short time, subsequently heated to the Ms point and holding for a specific time, and finally air cooled to the room temperature. It is found that the resulting multiphase microstructure consists mainly of prior lenticular martensite formed during controlled quenching (PM), needle bainitic ferrite (BF), and high carbon enriched retained austenite (RA). Further observation shows that a nanostructured (BF+RA)nano phase including lath BF and film RA with a width of about 100 nm nucleates around the PM. Such a microstructure results in uniform compression behavior, and significantly higher strength and hardness than for a conventional 60Si2Mn disc spring. This controlled multi-step austempering process is a promising solution for enhancing the disc spring properties for those applications involving higher loading and fatigue conditions

Liang, Z.[a] , Zhou, W.[a] , Wang, X.[a] , Northwood, D.O.[b] , Liu, C.[a]

A 2.1 GPA triple-phase spring steel
(2018) *WIT Transactions on the Built Environment*, 175, pp. 1-7.

DOI: 10.2495/HPSM180011

[a] College of Mechanical Engineering, Yangzhou University, China
[b] Mechanical, Auto and Materials Engineering, University of Windsor, Canada

Abstract
The key way of achieving sustainability of a product is to design a manufacturing process that increases the mechanical properties of traditional materials, e.g. steel, whilst also increasing processing efficiency, and diminishing energy consumption. A novel process has been developed that allows for a traditional spring steel (60Si2Mn) to be produced with a high level of strength (tensile strength is over 2100 MPa, bending strength is 4100 MPa, yield strength is 1700 MPa as well as hardness of 59 HRC), also retaining reasonable ductility on an industrial scale. It is shown that a triple-phase microstructure comprising lenticular prior martensite, nano-scaled needle/lath-like bainitic ferrite and film retained austenite, is obtained. The excellent combination of strength and ductility is attributed to a synergistic multi-phase strengthening effect. The nano-scaled structure exhibits a good balance between strength and toughness. The presence of prior martensite provides the kinetics of subsequent nano-scaled bainitic transformation by bainitic laths nucleating at the martensite–austenite interfaces. This design methodology potentially broadens the application of spring steel to components that experience more demanding service environments, such as heavy loads

Zhou, R., Northwood, D.O., Liu, C.

On nitrogen diffusion during solution treatment in a high nitrogen austenitic stainless steel
(2020) *Journal of Materials Research and Technology*, 9 (2), pp. 2331-2337.

Abstract
The generation and microstructural characteristics of the surface layer formed during solution treatment at 1200 °C of a high nitrogen austenitic stainless steel, have been investigated using optical microscopy, X-ray diffraction (XRD) and scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS). Contrasting with a bulk microstructure of austenite and ferrite, a multi-layer surface structure is obtained, which consists of a white outer-surface layer which is ferrite and a grey subsurface layer with austenite. Formation of the multi-layer structure occurs through phase transformations between austenite and ferrite due to the various levels of nitrogen diffusion. With increasing solution treatment time, the thicknesses of both the surface and the subsurface layer increase. Hardness tests show that the microhardness increases from the surface layer, to the subsurface layer and then to the bulk. This is attributed to the combined effects of solid solution strengthening from nitrogen and the grain size of austenite or ferrite.

2. Innovation in Engineering Education

In 2020, I have continued working with Associate Professor Daniela Pusca, University of Windsor, on the challenges we face as educators in an engineering faculty. C0VID-19 has presented its own challenges and has highlighted the need for change. Any change should be a "positive" change which will enhance the student experience and, ultimately, student success. We have identified three stages in the change process:

1. Initiation: Why is change important?
2. Implementation: How to achieve to change?
3. Sustaining: What are the elements of successful change?

High impact practices (HIPS) are identified as an important component of the implementation. We have examined two approaches for successful positive change, namely the change equation and appreciative inquiry. They differ in how they address the Why? The change equations starts with dissatisfaction and identifies what is "wrong". Appreciative inquiry, on the other hand, first of all identifies processes that work well now It does acknowledge that new situations do require change but any change must be consistent with the best of the previous practices. Related publications include:

Pusca, D., Northwood, D.O.

The impact of positive change in higher education
(2020) World Transactions on Engineering and Technology Education, 18(4), pp. 427-432

Abstract
In order to enhance the student experience and, ultimately, student success, there have been many calls for positive change in the quality of undergraduate education. These changes are being asked for at a time when universities are facing financial, and other, challenges. In this article, the authors examine how positive change can be achieved in undergraduate engineering programmes. Three stages are identified in the change process: initiating (Why is change important?); implementing (How to achieve change?); and sustaining (What are the elements of successful change?). High impact practices are identified as important components of quality undergraduate education (the How?). In examining elements for successful change, two approaches are discussed, the change equation and appreciative inquiry. The change equation starts with dissatisfaction as the Why? identifies what is wrong. Appreciative inquiry begins with discovery; it identifies processes that work well now. Through appreciative inquiry, there is an acknowledgement that new conditions exist that require change, but that any change must be consistent with the best of the old.

Pusca, D., Northwood, D.O.

The why, what and how of teaching: An engineering design perspective
(2017) *Global Journal of Engineering Education*, 19 (2), pp. 106-111.

University of Windsor, Windsor, ON, Canada

Abstract
The why, what and how of teaching are examined from the perspective of teaching engineering design in an integrative learning environment. Why is the guiding vision and relates to why one reads or studies particular topics. It is the starting point of the learning process. Once why has been established, a backward design approach is utilised to formulate the what and how. What relates to the development of discipline-specific skills and competencies. The what for engineering design is considered from the perspective of the ability to a) generate new design solutions; b)improve existing design solutions; and c) manage design. How is the creative strategy that effectively supportstransformative learning and can involve three other ws; namely, who, when and where. Successful engineering design education requires the active participation of students in all stages of the educational process.

Pusca, D., Northwood, D.O.

Implementation of high-impact practices in engineering design courses
(2018) *World Transactions on Engineering and Technology Education*, 16 (2), pp. 108-114. .

University of Windsor, Windsor, ON, Canada

Abstract
Teaching and learning practices have an impact on students' performance and their ability to achieve the required graduate attributes. Educational institutions are asked to consider practices that ensure both academic success in university and post-graduation outcomes in the workforce. As part of the institutional approach to innovation in teaching and learning excellence, engineering design courses were redesigned to improve student experience, and also to include more high-impact practices. This article examines the high-impact curricular practices that were implemented in engineering design courses as teaching practices, and how they relate to the desired learning outcomes. Student engagement is considered as a measure of effective learning. Using evidence, the authors argue that experiential learning and high-impact practices lead to greater engagement, better prepare students for future employment, and help to bridge acknowledged gaps between education and practice.

Pusca, D., Bowers, R.J., Northwood, D.O.

Hands-on experiences in engineering classes: The need, the implementation and the results
(2017) *World Transactions on Engineering and Technology Education*, 15 (1), pp. 12-18.

University of Windsor, Windsor, ON, Canada

Abstract
The mission and vision of engineering education should continuously change its focus to satisfy customers' requirements - the industry and the students as future employees. The main issue that needs to be addressed by faculty that teach undergraduate engineering courses is how well the graduate engineers are equipped with the practical skills required by industry. This article describes a systematic approach for introducing practical hands-on experiences in engineering courses. The case studies illustrate the implementation, the benefits and the results of this approach designed for student engagement. They will demonstrate the importance of considering both virtual materials and physical materials for hands-on activities, and to implement experiential activities that are employed by practicing engineers.

Scalable, Low-Temperature, Low Vacuum van der Waals Epitaxy of 2D Materials Using Atomic Layer Deposition

by Markku Leskelä, Member EUAS

Short Biography

Markku Leskelä *(born 1950), ORCID 0000-0001-5830-2800*
http://www.helsinki.fi/kemia/epaorgaaninen/personnel/leskela.htm
https://tuhat.helsinki.fi/portal/en/persons/markku-leskela(78010015-5f49-49b7-b712-54b1b327ac7b).html

Education and degrees completed

D. Techn. 1980, MSc 1974, Helsinki University of Technology

Current position

Professor emeritus, University of Helsinki

Previous work experience

PhD student Helsinki University of Technology (1973-1979); Associate professor University of Oulu (1979-1981; 1982-1986); Professor Helsinki University of Technology (1981-1982); Professor University of Turku (1986-1990); Professor University of Helsinki, 1990 – 2018; Academy professor 2004-2009

Research interests

Research activities include thin films and nanostructured materials made by various chemical methods (Atomic Layer Deposition, electrodeposition and Successive Ionic Layer Adsorption and Reaction) for applications in micro- and optoelectronics. The studies include all stages in film growth from precursor synthesis to applications. The other research topic is catalysis where the focus is in activation of small molecules by metal complexes in homogeneous systems. Co-author of 713 peer reviewed papers, 66 reviews and holder of 53 patents. Number of citations 26 600; h-index 74 (Web of Science)

Personal research funding

Number of research grants during whole carrier is about 80. Most important recent fundings:
Interfacial engineering of semiconductors for highly selective light-driven chemical transformations (Academy of Finland 2020-2023) 315 000€; European Research Training Network of Functional Hybrid Coatings by Molecular Layer Deposition (EU, 2017-2021) 538 000€; Finnish Centre of Excellence in Atomic Layer Deposition (Academy of Finland, University of Helsinki, 2015-2019) 2 920 000 €; Building-up Centre of Excellence for advanced materials, (EU Teaming project, 2015-16) 130 000 €; Development of ALD processes for microelectronic applications (ASM Microchemistry, 2014-2018) 1 300 000 €

Awards and honours

Member of Finnish Academy of Science and Letters 1991- ; Finnish Academy of Technical Sciences 1996-; Finnish Society of Sciences and Letters 2005-; SVR I 2005; Magnus Ehrnrooth Foundation Award 2002; ISI Highly cited scientist 2004-; A.I Virtanen award 2011; American Vacuum Society ALD award 2012; Award of Finnish Academy of Sciences and Letters 2014; Honorary member of Finnish Chemical Society 2014; Honorary doctor, University of Tartu 2016; Member of EU Academy of Sciences 2018

Other scientific or academic merits

Member of board of governors in University of Helsinki, 2010-2017; opponent for 35 PhD theses, pre-examiner for 37 PhD theses, referee for 30 professor positions, evaluator for research proposals in 14 countries, ca. 100 invited talks in international conferences, numerous positions in trust in Finnish and international scientific societies, editorial board member of 6 journals (1989-2019), board member of seven foundations (1992-2019).

Scalable, Low-Temperature, Low Vacuum van der Waals Epitaxy of 2D Materials Using Atomic Layer Deposition.

M. Mattinen, P.J. King, G. Popov, J. Hämäläinen, M.J. Heikkilä, M. Leskelä & M. Ritala

2D Materials 7 (2020) 011003 (7 pp.)

Van der Waals epitaxy holds great promise in producing high-quality films of 2D materials. However, scalable van der Waals epitaxy processes operating at low temperatures and low vacuum conditions are lacking. Herein, atomic layer deposition is used for van der Waals epitaxy of continuous multilayer films of 2D materials HfS_2, MoS_2, SnS_2, and ZrS_2 on muscovite mica and PbI_2 on sapphire at temperatures between 75 and 400 ^oC. For the metal sulfides on mica, the main epitaxial relation is MS_2 mica. Some domains rotated by 30 degrees are also observed corresponding to the MS_2 mica alignment. In both cases, the presence of domains rotated by 60 degrees (mirror twins) is also expected. For PbI_2 on sapphire, the epitaxial relation is PbI_2 Al_2O_3 with no evidence of 30 degrees domains. For all of the studied systems there is relatively large in-plane mosaicity and in the PbI_2/Al_2O_3 system some non-epitaxial domains are also observed. The study presents first steps of an approach towards a scalable and semiconductor industry compatible van der Waals epitaxy method.

Silicon Oxide -Niobium Oxide Mixture Thin Films Atomic and Nanolaminates grown by Layer Deposition from Niobium Pentaethoxide and Hexakis(ethylamino)disilane.

K. Kukli, M. Kemell, M.J. Heikkilä, H. Castán, S. Dueñas, K. Mizohata, M. Ritala & M. Leskelä

Nanotechnology 31 (2020) 195713 (10 pp).

Amorphous SiO_2-Nb_2O_5 nanolaminates and mixture films were grown by atomic layer deposition. The films were grown at 300 degrees C from $Nb(OC_2H_5)_5$, $Si_2(NHC_2H_5)_6$, and O_3 to thicknesses ranging from 13 to 130 nm. The niobium to silicon atomic ratio was varied in the range of 0.11-7.20. After optimizing the composition, resistive switching properties could be observed in the form of characteristic current-voltage behavior. Switching parameters in the conventional regime were well defined only in a SiO_2:Nb_2O_5 mixture at certain, optimized, composition with Nb:Si atomic ratio of 0.13, whereas low-reading voltage measurements allowed recording memory effects in a wider composition range.

Synthesis, Molecular Docking Studies, and Larvicidal Activity Evaluation of New Fluorinated Neonicotinoids against Anopheles darling Larvae.

R.S. Mesquita, A. Kyrylchuk, I. Grafova, D. Kliukovskyi, A. Bezdudnyy, A. Rozhenko,

W.P. Tadei, M. Leskelä & A. Grafov

PlosOne 15 (2020) e0227811 (20 pp.)

Anopheles darlingi is the main vector of malaria in Brazil, characterized by a high level of anthropophilia and endophagy. Imidacloprid, thiacloprid, and acetamiprid are the most widespread insecticides of the neonicotinoid group. However, they produce adverse effects on the non-target insects. Flupyradifurone has been marketed as an alternative to non-fluorinated neonicotinoids. Neonicotinoids containing trifluoroacethyl substituent reveal increased insecticidal activity due to higher hydrophobicity and metabolic stability. We synthesized novel neonicotinoid insecticides containing fluorinated acceptor groups and their interactions were estimated with the nicotinic acetylcholine receptor (nAChR) binding site by molecular docking studies, to evaluate their larvicidal activity against A. darlingi, and to assess their outdoor photodegradation behavior. New neonicotinoid analogues were prepared and characterized by NMR and mass-spectrometry. The synthesized molecules were modelled by time-dependent density functional theory and analyzed, their interaction with nAChR was investigated by molecular docking. Their insecticide activity was tested on Anopheles larvae collected in suburban area of Manaus, Brazil. Four new fluorinated neonicotinoid analogs were prepared and tested against 3(rd) instars larvae of A. darlingi showing high larvicidal activity. Docking studies reveal binding modes of the synthesized compounds and suggest that their insecticidal potency is governed by specific interactions with the receptor binding site and enhanced lipophilicity. 2-Chloro-5-(2-trifluoromethyl-pyrrolidin-1-ylmethyl)pyridine 5 showed fast degradation in water maintaining high larvicidal activity. All obtained substances possessed high larvicidal activity in low concentrations in 48 hours of exposure, compared to commercial flupyradifurone. Such activity is connected to a unique binding pattern of the synthesized compounds to insect's nAChR and to their enhanced bioavailability owing to introduction of fluorinated amino-moieties. Therefore, the compounds in question have a high potential for application as control agents for insects transmitting tropical diseases, and they will be less persistent in the environment.

Photocatalytic and Gas Sensitive Multiwalled Carbon Nanotube/TiO_2-ZnO and ZnO-TiO_2 Composites Prepared by Atomic Layer Deposition.

I.M. Szilágyi, L.P. Bakos, J. Nóra, U.C.M. da Silva Bezerra da Costa, K. László, J.L. Lábár, T. Igricz, K. Varga–Josepovits, P. Pasierb, E. Färm, M. Ritala, M. Leskelä & I.M. Szilagyi

Nanomaterials 10 (2020) 252 (14 pp.)

TiO_2 and ZnO single and multilayers were deposited on hydroxyl functionalized multi-walled carbon nanotubes using atomic layer deposition. The bare carbon nanotubes and the resulting heterostructures were characterized by TG/DTA, Raman, XRD, SEM-EDX, XPS,

TEM-EELS-SAED and low temperature nitrogen adsorption techniques, and their photocatalytic and gas sensing activities were also studied. The carbon nanotubes (CNTs) were uniformly covered with anatase TiO_2 and wurtzite ZnO layers and with their combinations. In the photocatalytic degradation of methyl orange, the most beneficial structures are those where ZnO is the external layer, both in the case of single and double oxide layer covered CNTs (CNT-ZnO and CNT-TiO_2-ZnO). The samples with multilayer oxides (CNT-ZnO-TiO_2 and CNT-TiO_2-ZnO) have lower catalytic activity due to their larger average densities, and consequently lower surface areas, compared to single oxide layer coated CNTs (CNT-ZnO and CNT-TiO_2). In contrast, in gas sensing it is advantageous to have TiO_2 as the outer layer. Since ZnO has higher conductivity, its gas sensing signals are lower when reacting with NH_3 gas. The double oxide layer samples have higher resistivity, and hence a larger gas sensing response than their single oxide layer counterparts.

X-ray Scattering and Morphological Studies of Atomic Layer Deposited IrO_2.

M.J. Heikkilä, J. Hämäläinen, E. Puukilainen, M. Ritala & M. Leskelä

Journal of Applied Crystallography 53 (2020) 369-380.

IrO_2 is an important material in numerous applications ranging from catalysis to the microelectronics industry, but despite this its behaviour upon annealing under different conditions has not yet been thoroughly studied. This work provides a detailed investigation of the annealing of IrO_2 thin films using in situ high-temperature X-ray diffraction and X-ray reflectivity (HTXRR) measurements from room temperature up to 1000 ^oC in oxygen, nitrogen, forming gas and vacuum. Complementary ex situ scanning electron microscopy and atomic force microscopy measurements were conducted. The combined data show the dependencies of crystalline properties and surface morphology on the annealing temperature and atmosphere. The reduction of IrO_2 to Ir takes place at a temperature as low as 150 ^oC in forming gas, but in oxygen IrO_2 is stable up to 800 ^oC and evaporates as a volatile oxide at higher temperatures. The IrO_2 crystallite size remains constant in oxygen up to 400 ^oC and increases above that, while in the more reducing atmospheres the Ir crystallites grow continuously above the phase-change temperature. The role of HTXRR in the analysis is shown to be important since its high sensitivity allows one to observe changes taking place in the film at temperatures much below the phase change.

Magnetic Properties and Resistive Switching in Mixture Films and Nanolaminates Consisting of Iron and Silicon Oxides Grown by Atomic Layer Deposition.

K. Kukli, M. Kemell, H. Castán, S. Dueñas, J. Link. R. Stern, M.J. Heikkilä, T. Jogiaas, J. Kozlova, M. Rahn, K. Mizohata, M. Ritala & M. Leskelä

Journal of Vacuum Science & Technology A 38 (2020) 042405 (11 pp.)

SiO_2-Fe_2O_3 mixture films and nanolaminates were grown by atomic layer deposition from iron trichloride, hexakis(ethylamino)disilane, and ozone at 300 ^oC. Orthorhombic -Fe_2O_3 was identified in Fe_2O_3 reference films and in Fe_2O_3 layers grown to certain thicknesses between amorphous SiO_2 layers. SiO_2-Fe_2O_3 films could be magnetized in external fields, exhibiting saturation and hysteresis in nonlinear magnetization-field curves. Electrical resistive switching, markedly dependent on the ratio of the component oxides, was also observed in films with proper composition. For relatively conductive films, application of small signal measurements allowed one to record memory maps with notable squareness and defined distinction between high and low conductance states.

Area-selective Molecular Layer Deposition of Polyimide on Cu through Cu-catalyzed Formation of a Novel Crystalline Interchain Polyimide.

Chemistry of Materials 32 (2020) 5073-5083.

C. Zhang, M. Vehkamäki, M. Pietikäinen, M. Leskelä & M. Ritala

Novel area-selective molecular layer deposition (AS-MLD) of polyimide (PI) on Cu versus native SiO_2 was studied. By use of 1,6-diaminohexane (DAH) and pyromellitic dianhydride (PMDA) as precursors, PI films can be selectively deposited on the Cu surface at 200-210 ^oC with a rate around 7.8 A/cycle while negligible growth takes place on SiO_2. The selectivity was successfully demonstrated also on Cu/SiO_2 patterns at 200 ^oC; after 180 MLD cycles, around 140 nm thick PI was deposited on Cu regions while <10 nm thick PI was measured on SiO2 regions. By contrast, at 170 ^oC, similar growth rates were measured on Cu (4 angstrom/cycle) and native SiO2 (5 angstrom/cycle). To understand the origin of the selectivity, properties of PI film grown on Cu at the selectivity enabling temperature of 200 ^oC have been thoroughly compared with those grown on both Cu and native SiO_2 at the nonselective temperature of 170 ^oC. Significant differences in crystallinity, surface morphology, and chemical structure suggest that the PI films grown on Cu at 200 ^oC have a novel crystalline interchain PI structure. According to this finding, the selectivity mechanism is proposed to derive from a new MLD reaction mechanism catalyzed by copper ions at 200-210 ^oC that leads to the formation of new crystalline polymer species. Additionally, it is suggested that small amounts of Cu ions can float on the surface of the growing PI film and thereby constantly catalyze the MLD reaction, as evidenced by XRD, XPS, and ToF-ERDA. The high catalytic efficiency has been also proven by using successfully an ultrathin Cu layer, nominally 0.1 nm, as a seed layer to initiate the MLD growth.

Scalable, Controlling the Growth of 2D Semiconductor SnS_2 bu the Choice of Substrate: Towards Monolayer Films and van der Waals Epitaxy.

M. Mattinen, P.J. King, M. Leskelä & M. Ritala

Applied Materials & Interfaces 7 (2020) 2001046 (10 pp).

Semiconducting 2D materials, such as SnS_2, hold great promise in a variety of applications including electronics, optoelectronics, and catalysis. However, their use is hindered by the scarcity of deposition methods offering necessary levels of thickness control and large-area uniformity. Herein, a low-temperature atomic layer deposition (ALD) process is used to synthesize up to 5x5 cm^2continuous, few-layer SnS_2 films on a variety of substrates, including SiO_2/Si, Si-H, different ALD-grown films (Al_2O_3, TiO_2, and Ir), sapphire, and muscovite mica. As a part of comprehensive film characterization, the use of low energy ion scattering (LEIS) is showcased to determine film continuity, coverage of monolayer and multilayer areas, and film thickness. It is found that on sapphire substrate, continuous films are achieved at lower thicknesses compared to the other substrates, down to two monolayers or even less. On muscovite mica, van der Waals epitaxial growth is realized after the post-deposition annealing, or even in the as-deposited films when the growth is performed at 175 to 200 ^oC. This work highlights the importance of the substrate choice for 2D materials and presents a practical low-temperature method for the deposition of high-quality SnS_2 films that may be further evaluated for a range of applications.

Atomic Layer Deposition of PbS Thin Films at Temperatures below 100 ^oC for Halide Perovskites.

G. Popov, G. Bacic, M. Mattinen, T. Manner, H. Lindström, H. Seppänen, S. Suihkonen, M. Vehkamäki, M. Kemell, P. Jalkanen, K. Mizohata, J. Räisänen, M. Leskelä, H. Koivula, S. Barry & M. Ritala

Chemistry of Materials 32 (2020) 8216-8228.

Atomic layer deposition (ALD) is a viable method for depositing functional, passivating, and encapsulating layers on top of halide perovskites. Studies in that area have only focused on metal oxides, despite a great number of materials that can be made with ALD. This work demonstrates that, in addition to oxides, other ALD processes can be compatible with the perovskites. We describe two new ALD processes for lead sulfide. These processes operate at low deposition temperatures (45-155 ^oC) that have been inaccessible to previous ALD PbS processes. Our processes rely on volatile and reactive lead precursors Pb(dbda) (dbda = rac-N_2,N_3-di-tertbutylbutane-2,3-diamide) and $Pb(btsa)_2$ (btsa = bis(trimethylsilyl)amide) as well as H_2S. These precursors produce high quality PbS thin films that are uniform, crystalline, and pure. The films exhibit p- type conductivity and good mobilities of 10-70 $cm^2\ V^{-1}\ s^{-1}$. Low deposition temperatures enable direct ALD of PbS onto a halide perovskite $CH_3NH_3PbI_3$ (MAPI) without its decomposition. The stability of MAPI in ambient air is greatly improved by capping with ALD PbS. More generally, these new processes offer valuable alternatives for PbS-based devices, and we hope that this study will inspire more studies on ALD of non-oxides on halide perovskites.

Systematic Non-dimensional Parametric Investigation for the Thermo-fluid Dynamics of Two-layered Fluid Systems

by William M. Worek, Member EUAS

Short Biography

EDUCATIONAL BACKGROUND

- *Ph.D. Mechanical and Aerospace Engineering, Illinois Institute of Technology, 1980.*
- *M.S. Mechanical and Aerospace Engineering, Illinois Institute of Technology, 1977.*
- *B.S. High Honors, Mechanical Engineering, Illinois Institute of Technology, 1976.*

ADMINISTRATIVE EXPERIENCE

- *November 2017 – present*
  Professor, Mechanical and Industrial Engineering, Texas A&M – Kingsville.
- *January 2016 – October 2017*
  Executive Director, Eagle Ford Center for Research Education and Outreach and Professor, Mechanical Engineering, Texas A&M – Kingsville.
- *September 2013 – December 2105*
  Professor and Associate Dean Research and Graduate Studies, Stony Brook University.
- *July 2012 – May 2013*
  Dave House Professor and Dean of Engineering, Michigan Technological University.
- *August 2000 – July 2009*
  Head, Department of Mechanical Engineering, University of Illinois at Chicago.
- *October 2000 – September 2010*
  Director, UIC Industrial Assessment Center, U.S. Department of Energy.
- *August 1999 – July 2000*
  Interim Head, Department of Mechanical Engineering, University of Illinois at Chicago
- *August 1998 – January 2009*
  Director, Energy Resources Center, University of Illinois at Chicago.
- *September 1995 – August 1999*
  Associate Department Head, Department of Mechanical Engineering, University of Illinois at Chicago.

PROFESSIONAL EXPERIENCE

- *August 2013 – preset, Professor, Department of Mechanical Engineering, Stony Brook University.*
- *July 2012 – May 2013, Professor, Department of Mechanical Engineering – Engineering Mechanics, Michigan Technological University.*
- *September 1995 – July 2012, Professor, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *September 1989 – August 1995, Associate Professor (tenured), Department of Mechanical Engineering, University of Illinois at Chicago.*
- *September 1986 – 1989, Associate Professor, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *August 1980 – August 1986, Assistant Professor, Department of Mechanical and Aerospace Engineering, Illinois Institute of Technology.*
- *August 1978 – August 1980, Part–Time Instructor (as a M.S. Graduate Student), Department of Mechanics, Mechanical and Aerospace Engineering, Illinois Institute of Technology.*
- *August 1977 – August 1978, Instructor, Department of Mechanics, Mechanical and Aerospace Engineering, Illinois Institute of Technology.*

UNIVERSITY SERVICE

- *2013 – 2015, Faculty Leadership Team, SUNY – Research Foundation Energy, Environment, Economics, Education (4E) Network of Excellence.*
- *2008 – 2012, Chancellor's Committee on Sustainable and Energy, University of Illinois at Chicago.*
- *2007– 2012, University of Illinois (all campuses), Energy Committee.*
- *2001 – 2002, Academic Leadership Program, One of four UIC members, Committee on Institutional Cooperation, University Memberships include: University of Chicago, University of Illinois, Indiana University, University of Iowa, University of Michigan, Michigan State University, University of Minnesota, Northwestern University, Ohio State University, Pennsylvania State University, Purdue University, University of Wisconsin – Madison.*
- *1995 – 1999, Elected Member, College of Engineering Executive Committee, University of Illinois at Chicago.*
- *1995 – 1997, Chair, Faculty Search Committee, Department of Mechanical Engineering, The University of Illinois at Chicago.*
- *1996 – 1997, Member, Civil and Materials Engineering Department Head Review Committee, College of Engineering, University of Illinois at Chicago.*
- *1995 – 1996, Chair, Chemical Engineering Department Head Search Committee, College of Engineering, University of Illinois at Chicago.*
- *1994 – 1999, Elected Member, Department of Mechanical Engineering Advisory Committee, University of Illinois at Chicago.*
- *1993 – 1994, Chair, College of Engineering Educational Policy Committee, University of Illinois at Chicago.*
- *1993 – 1994, Elected Member, Department of Mechanical Engineering Advisory Committee, University of Illinois at Chicago.*
- *1992 – 1994, Chair, College of Engineering–Nominating Committee for the University Teaching Award, University of Illinois at Chicago.*
- *1989 – 1992, Director of Graduate Studies, Department of Mechanical Engineering, University of Illinois at Chicago.*
- *1989 – 1991, Chair, College of Engineering, Educational Policy Committee, University of Illinois at Chicago.*

RESEARCH INTERESTS

Heat and mass transfer, fluid flow, thermodynamics as applied to energy efficient, renewable and sustainable energy systems. Single and multicomponent absorption and adsorption processes in liquid and solid desiccants, heating and cooling components and systems. Energy policy factors that impact implement of energy systems, energy utilization and energy procurement.

RESEARCH SUPPORT

Professor Worek has received over USD$18M in support of his research. Sponsors have included: U.S. Department of Energy, U.S. Department of Defense, EnergTek, Commonwealth Edison, Tennessee Valley Authority, LaRoche Chemicals, Kaiser Chemicals, the Gas Research Institute, Englehard/ICC, John Crane, Telaire Systems, AEC, Hoechst-Celanese, Oak Ridge National Laboratory, Brookhaven National Laboratory, Ebara Research, Institute of Gas Technology, Munters/Cargocaire, Semco, N-Baro Tech., Blue Moon Fund, and the National Center for Energy Management and Building Technology.

AWARDS

- *Frank Kreith Energy Award, November 2018 (Honoring individuals for significant contributions to a secure energy future with particular emphasis on innovations in conservation and/or renewable energy) – Awarded at the American Society of Mechanical Engineers (ASME) – International Mechanical Engineering Congress and Exhibition (IMECE) Meeting – once per year.*
- *Edwin F. Church Award, 2013 ASME (Established in 1972 to honor individuals for distinguished service to mechanical engineering education in activities other than teaching, research and administration) – Awarded at the ASME IMECE Meeting – once per year.*
- *ASME Distinguished Service Award, 2013.*
- *Fellow, American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE), 2012.*
- *Nominated for UIC Excellence in Teaching Award, 2003 (a UIC Campus-wide Award).*
- *Harold A. Simon Award for Excellence in Teaching, 2000 (a UIC-College of Engineering Award).*
- *Fellow, American Society of Mechanical Engineers (ASME), 2001.*
- *University of Illinois, Committee on Institutional Cooperation (CIC) Academic Leadership Program (ALP) Fellow, 2001–2002.*

Systematic non-dimensional parametric investigation for the thermo-fluid dynamics of two-layered fluid systems

Abstract

Fluid dynamics and heat transfer of immiscible two-layered fluid systems have been of great importance in a variety of industrial as well as extraterrestrial exploration applications. Control and optimization of such a liquid-liquid arrangement need complete understanding of complex synergistic phenomena, especially those induced by surface tension at the fluid interface. Previously-reported investigations for the natural and Marangoni convection of two-layered immiscible systems have been incoherent, having no systematic presentation based on the key dimensionless parameters that govern the flow. The paper here presents a rigorous scheme and the results of a non-dimensional analysis, which allows a systematic and coherent interpretation of the system flow. The approach leads to ten non-dimensional parameters to completely characterize the thermo-fluid dynamics under the hypothesis of flat non-deformable interface. The system for a set of dimensionless parameters can have five degrees of freedom in physical variables, with fifteen dimensional physical variables appearing in the governing equations. The effect and importance of each non-dimensional parameter have also been numerically analyzed in search of a further reduction of the parameters describing the phenomena. © 2012 Elsevier Ltd. All rights reserved.

Comparison study of the counter-flow regenerative evaporative heat exchangers with numerical methods

Abstract

This paper numerically investigates the performance and heat and mass transfer processes that occur in regenerative heat and mass exchangers (HMXs) used for indirect evaporative air cooling. Two basic types of regenerative air coolers were compared: an exchanger with typical airflows arrangement and an exchanger with perforations along the whole length of the dry channel. The numerical model is based on one-dimensional heat and mass transfer assumptions and was validated against existing experimental data. The results obtained from the simulation reveal high effectiveness of the presented unit. The results allow defining optimal geometric and operational parameters for the typical regenerative exchanger and regenerative exchanger with perforations. It was determined that the value of working to main air-flow ratio has a significant impact on the cooling performance of considered air coolers. © 2015 Elsevier Ltd. All rights reserved.

Comparative analysis between traditional and M-Cycle based cooling tower

Abstract

The following paper presents the first numerical comparison of heat and mass transfer processes in a traditional cooling tower and a solution based on the

Maisotsenko cycle (M-Cycle). The results of the simulation allowed us to analyze the heat and mass transfer process occurring inside the M-Cycle and the traditional cooling tower and to observe its most important characteristics and features. The analysis was performed for two hypothetical situations: 1) both towers having the same external dimensions: the Number of heat Transfer Units (NTU) of M-Cycle cooling tower was two times smaller, due to its geometry; 2) two towers have the same mass transfer surface (i.e. identical NTU in wet channels). It was confirmed that M-Cycle Cooling Tower (MCT) can cool the water below the wet-bulb temperature (which is not achievable by conventional cooling towers), even in very hot and humid conditions (outdoor air temperature of 40 °C and humidity ratio of 20 g/kg). Also, the influence of the selected parameters (including inlet air temperature and humidity, inlet water temperature, NTU, and heat capacity ratio between water and air) on cooling tower performance are documented. Critical factors which have the highest impact on its effectiveness are established and discussed. The study confirmed high practical potential of using M-Cycle in water cooling applications. © 2020 Elsevier Ltd

Falling-film thermosyphons: Application to water harvesting from humis gas streams

Abstract

Water harvesting from humid gas streams is central to fresh-water production, desalination, and particulate removal from combustion gas streams. Two-phase thermosyphons are well suited for these applications due to their very low thermal resistance, but have several operating limits at the high heat flows required for such applications. This work introduces the falling-film thermosyphon for large-scale condensation applications. Working fluid is pumped to the top of the evaporator to provide the evaporating liquid film on the inner tube wall, rather than by vapor condensation. The flooding, dry-out and pool-boiling limits are eliminated, resulting in significantly higher maximum heat fluxes for the same physical evaporator size. Additionally, the condenser no longer needs to be located vertically above the evaporator, which allows for a standard steam condenser to be used. A model for the condensation process in humid air was developed that estimates the fluid and heat transfer and is confirmed experimentally. Other benefits include the use of a high-thermal-conductivity polymer material for the evaporator section to minimize corrosion, and the ability to impose a temperature boundary condition on the evaporator, which is made possible due to the elimination of a liquid pool. © 2020

Glacier-Related Outburst Floods

by John J. Clague, Member EUAS

Short Biography

Professor Emeritus
Simon Fraser University

Educational Background

1973 Ph.D. Geology, University of British Columbia, Canada
1969 M.A. Geology, University of California, United States
1967 A.B. Magna cum Laude, Geology, Occidental College, United States

Employment History

2003 - 2016 *Canada Research Chair in Natural Hazard Research, Earth Sciences, Simon Fraser University*
1998 - 2016 *Professor and Shrum Chair, Earth Sciences, Simon Fraser University, Burnaby BC*
1996 - 1998 *Adjunct Professor, Earth Sciences, Simon Fraser University, Burnaby BC*
1992 - 1998 *Senior Research Scientist, Geological Survey of Canada*
1988 - 1992 *Editor in Chief, Canadian Journal of Earth Sciences, National Research Council of Canada*
1986 - 1994 *Adjunct Professor, Institute for Quaternary Research, Simon Fraser University, Burnaby BC*
1974 - 1992 *Research Scientist, Geological Survey of Canada*
1973 - 1974 *NSERC Postdoctoral Fellow, Geological Survey of Canada*
1969 - 1970 *Teaching Assistant, Geological Sciences, University of British Columbia, Vancouver BC*

Research Specializations

Climate and environment change
Natural hazards and risk
Earthquake and tsunami history of southwestern British Columbia
Quaternary geology, Canada, Patagonia, European Alp, Southern Alps

Awards, Honors, and Scholarships

2020 *Officer, Order of Canada*
2020 *Soloviev Medal, European Geosciences Union*
2019 *Canadian Professional Geoscientist Professional Award, Geoscientists Canada*
2017 *Honorary PhD, University of Waterloo*
2012 *J. Willis Ambrose Medal, Geological Association of Canada, for sustained dedicated service to the Canadian earth science community*
2007 *Richard Jahns Distinguished Lecturer, Association of Engineering Geology, Geological Society of America, lectures at universities and earth science professional organizations throughout the Untied States and Canada*
2007 *Logan Medal, Geological Association of Canada, for outstanding contributions to earth science*
2006 *E.R. Ward Neale Medal, Geological Association of Canada, for exemplary contributions in earth science education in Canada*
2005 *Innovation 2005 Editorial Board Award, Association of Professional Engineers and Geoscientists of BC*
award for article "Could it happen in BC? Implications of the South Asia tsunami", published in Innovation
2003 *Canada Research Chair Tier I, Canada Research Chairs Secretariat, Government of Canada*

2002 *Bancroft Award, Royal Society of Canada, publication, instruction, and research in the earth sciences that have contributed to public understanding and appreciation of the subject*

2001 *Innovation 2001 Editorial Board Award, Association of Professional Engineers and Geoscientists of BC*
award for article "The Nisqually Earthquake: A wakeup call from south of the border", published in Innovation

1999 *Christopher J. Westerman Memorial Award, Association of Professional Engineers and Geoscientists of British Columbia, APEGBC's primary award for professional geoscience*

1998 *Fellow, Royal Society of Canada*

1995 *W.A. Johnston Medal, Canadian Quaternary Association, for excellence in Quaternary research*

1992 *Invited to give keynote address at MIT-sponsored Conference on Natural Hazards and Climate Change, Cambridge, Massachusetts*

1988 *E.B. Burwell, Jr. Memorial Award, Geological Society of America, for distinguished contribution to engineering geology*

1982 *Honorable Mention for best geotechnical paper in Canada, Canadian Geotechnical Society, paper published in Canadian Journal of Earth Sciences in 1982*

1982 *Award of Excellence, Society for Technical Communication, for paper published in Geos in 1982*

1966 *Elected to Phi Beta Kappa (U.S. national honorary society*

Career Accomplishments and Impact

John Clague is a leading authority in environmental earth sciences and climate change. He has made major contributions in geologic mapping, engineering and environmental interpretations of surficial geological information, and understanding natural hazards and risk. He is noted for local, national, and international research collaboration with geologists, geographers, biologists, and physicists. Clague has performed innovative research on the earthquake and tsunami hazards in southwestern British Columbia; his work has been a catalyst for earthquake research carried out by government, university, and private-sector scientists in Canada. He and his students have also conducted research on landslides, floods, and other natural hazards in Canada, USA, Bolivia, Argentina, Chile, Austria, Italy, and New Zealand. A major focus of his research, over the 47-year period since he published his first paper on large slumps in Point Reyes National Seashore in California, is landslides.

Clague has increased public and government awareness of natural hazards in western Canada by extensively publishing and lecturing on earthquakes, landslides, floods, and sea-level rise, and by advising decision makers in government and industry on these phenomena. He has published popular books on earthquakes, tsunamis, and other earth science issues in British Columbia, as well as a textbook on natural hazards that was widely adopted by Canadian universities.

Clague also pioneered efforts by the Geological Survey of Canada to make earth science information more accessible to the public. He conceived and produced innovative posters, maps, and other materials that communicate local geoscience knowledge to the public. These products led to similar efforts at communicating earth science issues outside the federal government.

Clague is author of nearly 300 peer-reviewed papers, reports, and monographs on a wide range of earth science topics of regional and national importance. He has given hundreds of television and radio interviews (CBC Newsworld, CBC Radio, CTV Television, Global TV, Weather Network) and newspaper and magazine articles (*Vancouver Sun, Victoria Times-Colonist, Toronto Star, Equinox, Beautiful B.C., Westside News, The Westerly News*). His research on earthquakes and tsunamis on the west coast of Canada was featured in a 1997 Discovery Channel documentary. A 2004 Discovery Channel documentary featured Clague's research on landslides. Clague has influenced Quaternary scientists in the United States and Europe; research on earthquakes, landslides, and floods has greatly increased public and official awareness of these hazards. He given more than 400 lectures at several North American universities, professional meetings, and public venues, and reviewed hundreds of papers for scientific journals.

Clague has received numerous awards for his research and outreach, including the GSA EB Burwell, Jr. Memorial Award for distinguished contribution to engineering geology. Clague was the Richard Jahns Distinguished Lecturer for the Association of Engineering Geology and Geological Society of America in 2007. He is recipient of several medals from the Geological Association of Canada, including the Logan Medal, its highest award. He is a past President of the Association of Professional Engineers and Geoscientists of British Columbia (APEGBC), only the third geoscientist to hold this position in the association's 95-year history. He a former President of the Geological Society of Canada, a former President of the International Union for Quaternary Research, and, since 1998, a Fellow of the Royal Society of Canada.

In 2013 and 2014, Clague served as Chair of a government-appointed Expert Review Panel on Landslide Hazard and Risk Assessment of the Cheekye River and Fan. In 2017, he served as a member of a three-person committee struck by the University of Toronto Scarborough to review the undergraduate program in the Department of Physical and Environmental Sciences. He previously served on a similar committee formed to evaluate undergraduate and graduate programs at the St. George campus of the University of Toronto. In 2013, Clague served as chair of two site-visit committees tasked with evaluating two national research projects funded by the Natural Sciences and Engineering Research Council (NSERC), one at Western University and the other at the University of British Columbia.

Clague was a member of an expert team assembled by BC Hydro and Power Authority to characterise seismic hazards to BC Hydro reservoirs and other assets. He prepared reports on tsunami hazards and risk for the District of North Vancouver and the Corporation of Delta. He consulted for a company tasked with evaluating the suitability of a proposed LNG facility on Ridley Island. He has consulted extensively on geological and engineering geological issues for municipal governments and private sector companies. Recent examples are consulting related to 1) several existing and proposed mining tailing storage facilities in British Columbia, and 2) large proposed water-supply infrastructure projects in the Metro Vancouver area.

Glacier-related outburst floods

John J. Clague, Jim E. O'Connor

Abstract

Water bodies impounded by glaciers, moraines, and ice jams on rivers can drain suddenly, with disastrous downstream consequences. Lakes can form at the margins of an alpine glacier or ice cap, on its surface, or at its base. Smaller pockets of water may also be present within some glaciers. In all cases, these water bodies might drain by enlarging subglacial tunnels or by mechanical collapse of the glacier dam. Many formerly stable glacier lakes have failed over the past century, in some cases repeatedly, as Earth's atmosphere has warmed and glaciers thinned and receded. The peak discharge, duration, and volume of a subglacial outburst flood depends mainly on the (1) geometry and rate of development of the tunnel at the base of the glacier, and (2) size and geometry of the impounded water body. Discharge commonly increases exponentially during the outburst, but ends quickly when the lake empties or when the drainage tunnel is plugged by collapse of the tunnel roof or closes due to plastic ice flow. Some glacier outburst floods result from the mechanical collapse of the ice dam. In such cases, the peak flow is achieved rapidly during the collapse. Outburst floods from glacier lakes attenuate due to temporary storage of floodwaters in channels and on valley floors.

Many hazardous lakes are dammed by lateral and end moraines that formed in the past two centuries when valley and cirque glaciers retreated from advanced positions reached during the Little Ice Age. Moraine dams are susceptible to failure because they are steep and relatively narrow, because they comprise loose poorly sorted sediment, and because they may contain ice cores or interstitial ice. These dams generally fail by overtopping and incision. The triggering event may be a heavy rainstorm, strong winds, or an ice avalanche or landslide into the lake that generates waves that overtop the dam. Melting of moraine ice cores and piping are other possible failure mechanisms. Outflow from a moraine-dammed lake increases as the breach enlarges and then decreases as the level of the lake falls. The moraine breach may become armored, preventing further incision, or the hydraulic gradient at the breach may decrease to a point that erosion ceases.

Outburst floods from glacier- and moraine-dammed lakes typically entrain, transport, and deposit large amounts of sediment. If the channel is steeper than about 0.10-0.15 and contains abundant loose sediment, the flood likely will transform into a debris flow. Such flows may be larger and more destructive than the flood from which they formed. A period of protracted warming is required to trap lakes behind moraines and create conditions that lead to dam failure. The warming also forces glaciers to retreat, prompting ice avalanches, and landslides that have destroyed many moraine dams.

A huge flood in the Fraser River valley, British Columbia, near the Pleistocene Termination

John J. Clague, Nicholas J. Roberts, Brendan Miller, Brian Menounos, Brent Goehring

Abstract

Near the Pleistocene Termination, a glacier-dammed lake in central British Columbia suddenly drained to the south along the Fraser River valley. Floodwater travelled 330 km down the valley to Hope, British Columbia, and from there to the west into the Salish Sea near Vancouver. The flood was caused by the failure of an ice dam formed by the terminus of glaciers flowing from the central Coast Mountains across the British Columbia Interior Plateau. The ice dam impounded several hundred cubic kilometres of water to a maximum elevation of about 810 m asl (above sea level); at its maximum, the lake at the ice dam was over 250 m deep. Geomorphic and sedimentary evidence for the flood includes streamlined boulder-strewn bars, gravel dune fields, and terraces sloping up Fraser and lowermost

Thompson valleys, opposite the present direction of current river flow. The gravel bars and flood terraces are underlain by sheets of massive to poorly sorted gravel containing large boulders and rip-up clasts of silt and till. Shortly after the flood, a landslide near the northern margin of the former glacier dam impounded water to an elevation of about 550 m asl. This lake emptied due to overflow and incision of the landslide dam. The outburst flood from glacial Lake Fraser and the subsequent draining of the landslide-dammed lake deeply incised the older sediment fill in Fraser Valley and transported much of this sediment into the proto-Salish Sea west of Vancouver, British Columbia and Bellingham, Washington. TCN ages on flood-transported boulders at three localities along the flood path agree with radiocarbon ages on inferred flood layers in ODP cores collected from Saanich Inlet, a fiord on southern Vancouver Island, 80 km south-southwest of Vancouver.

New Aspects of Relativistic Molecular Quantum Mechanics

by Wenjian Liu, Member EUAS

Short Biography

Education Background:

1. *Sept., 1992-July, 1995, Ph. D, Peking University, Beijing*
2. *Sept., 1989-July, 1992, M. Sc., Shandong University, Jinan*
3. *Sept., 1985-July, 1989, B. Sc., Shandong University, Jinan*

Work Experience:

1. *Dec., 2018-present, Shandong University, Chair Professor, inaugural director of Qingdao Institute for Theoretical and Computational Sciences*
2. *Dec., 2001-Dec., 2018, Cheung Kong Professor, Peking University*
3. *Jan., 1998-Dec., 2001, postdoc, Ruhr-Universität Bochum, Germany*
4. *Sept., 1995-Dec., 1997, postdoc, Max-Planck-Institut für Physik komplexer Systeme, Germany*

Academic Distinctions:

1. *Fellow of International Association of Advanced Materials (2020)*
2. *Vebleo fellow of molecular science (2020)*
3. *Fellow of Royal Society of Chemistry (2019)*
4. *Member of European Academy of Sciences (2019)*
5. *Fellow of Asia-Pacific Association of Theoretical and Computational Chemists (2017)*
6. *Fukui Medal of Asia-Pacific Association of Theoretical and Computational Chemists (2017)*
7. *Member of International Academy of Quantum Molecular Science (2014)*
8. *Bessel Award of the Humboldt Foundation (2007)*
9. *Annual Medal of International Academy of Quantum Molecular Science (2006)*
10. *Pople Medal of Asia-Pacific Association of Theoretical and Computational Chemists (2006)*
11. *Outstanding Young Scientist Award of National Natural Science Foundation (2006)*
12. *Cheung Kong Scholarship, State Education Ministry of China (2001)*
13. *QSCP (Quantum Systems in Chemistry and Physics) Promising Scientist Prize of CMOA (Centre de Mécanique Ondulatoire Appliquée), Europe, 2001*

Specializations

quantum electrodynamics, relativistic quantum chemistry, relativistic electronic structure theory, relativistic many-electron Hamiltonians, relativistic many-electron wave functions, relativistic time-dependent density functional theory, relativistic theories of magnetic properties, relativistic energy band theory, time-dependent density functional theory for nonadiabatic couplings between excited states, many-body theory for strongly correlated electrons, solvers for exterior/interior solutions of large eigenvalue problems

Scientific Achievements

Dr. Liu has long been working in the field of relativistic quantum chemistry, focusing mainly on methodological developments and programming. His achievements include (1) a series of relativistic many-electron Hamiltonians (eQED, Q4C, X2C, spf-X2C+soc-DKHn/BSSn/X2Cn) for electronic structure calculations of heavy elements; (2) a body-fixed four-component relativistic molecular Hamiltonian for spectroscopies involving the nuclear degrees of freedom; (3) four-component and exact two-component relativistic

theories of nuclear magnetic shieldings (4C/X2C-NMR) that capture naturally the diamagnetism missed in the standard relativistic linear response theory; (4) several variants of time-dependent density functional theory (4C/X2C-TD-DFT, spin-adapted open-shell TD-DFT, linear scaling TD-DFT, NAC-TD-DFT for nonadiabatic couplings between excited states); (5) a series of novel wave function-based correlation methods (SDSPT2, SDSCI, iCI, iCIPT2) for strongly correlated electrons; (6) an exact two-component relativistic energy band theory that provides absolute positions of energy bands; (7) a very efficient and robust solver for exterior or interior solutions of large eigenvalue problems; (8) the BDF program package for relativistic electronic structure calculations.

New Aspects of Relativistic Molecular Quantum Mechanics

The mathematical structure of the many-electron Schrödinger equation (SEQ) has long been known, viz. the Schrödinger-Coulomb (SC) Hamiltonian is self-adjoint and bounded from below, while the wave function is continuous and satisfies the SEQ locally everywhere. As such, what one needs to do is just to design various Ansätze (methods) to model the wave function, so as to solve the SEQ as accurately and efficiently as possible. However, the situation changes dramatically when we come back to the real world where light travels at a constant, finite speed (ca.137 a.u. or 300,000 km/s). The central questions are:

What equation is to be solved? How to solve it?

More specifically, the following questions must be addressed properly:

1. What is the appropriate (most accurate) relativistic many-electron Hamiltonian?
2. Is the Hamiltonian self-adjoint? Does it have bound states? But, are these relevant? That is, even if the Hamiltonian is self-adjoint and does have bound states, can the resulting equation be solved in the same way as the SEQ?
3. When is the no-pair approximation safe? If so, is it possible to make no-pair four- and two-component relativistic theories completely equivalent?
4. How to fuse relativistic quantum chemistry (RQC) and quantum electrodynamics (QED), the as yet two mutually exclusive subfields for electronic structure, so as to establish a continuous and complete field of relativistic molecular quantum mechanics (RMQM)?
5. How to derive a body-fixed relativistic molecular Hamiltonian for spectroscopies involving nuclear degrees of freedom?
6. How does the relativistic wave function behave at the coalescence of two electrons? How to do relativistic explicit correlation?
7. How to formulate relativistic properties that sample the electronic wave function in the vicinity of a nucleus?

These are the most general and fundamental issues concerning the three components (i.e., Hamiltonian H (Q1 to Q5), wave function Ψ (Q6), and energy/property $E(\lambda)$ (Q7) of the relativistic quantum mechanical equation $H\Psi = E\Psi$. Due to shortage of space, we can only summarize the essentials here.

(1) Relativistic Hamiltonians

Quantum electrodynamics (QED) is undoubtedly the highest level of theory for electromagnetic interactions between charged particles (nuclei, electrons, and positrons). However, full QED can nowadays be applied only to single ions of at most 5 electrons. To extend QED to many-electron atoms and molecules, in which correlation effects dominate over QED effects, we introduced an effective QED (eQED) approach[1-3] in a bottom-up fashion, i.e., without recourse to QED itself at all. For the same second order energy, eQED requires only three Goldstone diagrams but the standard formulation of QED has to take 28 Feynman diagrams. The former can readily go to higher orders whereas the latter suffers from too numerous diagrams. In short, eQED not only extends the applicability of QED from few- to many-electron systems, but also paves a seamless bridge between relativistic quantum chemistry and full QED[2-5]. Starting from eQED, various simplified no-pair relativistic Hamiltonians [quasi-4-component (Q4C)[4], exact two-component (X2C)[5-7], spin-separated X2C (sf-X2C+soc-DKHn/BSSn/X2Cn)[8,9], etc.] can be derived based solely on physical arguments. Together with other nonrelativistic and relativistic Hamiltonians, they form a complete and continuous "Hamiltonian Ladder"[10,11], from which one can pick up the right Hamiltonian according to the target physics and accuracy. In essence, relativistic Hamiltonians can only be formed in Fock space, whereas all first-quantized Hamiltonians suffer from the contamination of negative energy states[12], such that the corresponding QM equations cannot be solved in the same way as the SEQ. Instead, the no-pair approximation to first-quantized relativistic QM equations must be adopted from the outset. On the other hand, no-pair four- and two-component relativistic calculations can be and have been made completely equivalent in all aspects of simplicity, accuracy and efficiency[4]. For more thorough discussions see the comprehensive reviews[10,11,13,14,15,16].

(2) Relativistic Wave Functions

It has long been known that the exact wave function of the many-electron SEQ has cusps at the coalescence of two electrons, which cannot be modeled by orbital products (Slater determinants). As a direct consequence, electron correlation energies calculated by orbital-based methods converge extremely slowly with respect to the basis set size. The situation can only be improved by using explicitly correlated trial wave functions that depend explicitly on the interelectronic distances. Due to the interplay between relativity and correlation, electron correlation energies converge even slower in the relativistic regime. To resolve this issue, we analyzed in depth the structure of relativistic wave functions by making full use of the internal symmetry of reduced two-electron relativistic Hamiltonians[15] and thereby established the general framework for relativistic explicitly correlated wave function methods[14,17].

Apart from the slow convergence of the calculated correlation energy with respect to one-particle basis sets, how to parametrize many-electron wave functions is more intriguing, especially for strongly correlated systems of electrons featuring either multiple open-shell orbitals or nearly degenerate states, thanks to the existence of a dense set of energetically adjacent frontier orbitals. The common paradigm for treating such systems is to decompose the overall correlation into static and dynamic components and treat them differently. All the wave function-based methods can then be classified into three families: "static-then-dynamic", "dynamic-then-static" and "static-dynamic-static" (SDS)[18]. A series of novel wave function-based correlation methods can be stimulated from the generic SDS framework[18], including SDSCI[18],

SDSPT2[18,19], iCI[20], iCIPT2[21,22], etc., which all feature the construction and diagonalization of a small 3Np-by-3Np Hamiltonian matrix for Np target states, regardless of how many orbitals and how many electrons are to be correlated. All these methods can be combined with the relativistic Hamiltonians and relativistic explicit correlations for high-precision calculations of atoms and molecules.

(3) Relativistic Properties

Among others, nuclear magnetic shielding is a prototypical all-electron, relativistic property since it samples the electronic wave function in the vicinity of the nuclear position. Due to the fact that the Dirac operator is only linear with respect to magnetic fields, the standard four-component relativistic linear response theory of NMR shielding has only one term, the so-called paramagnetic term. That is, the familiar diamagnetic term known from nonrelativistic NMR theory[23] is `missing'. This is not only a conceptual problem but also a computational problem: The computation is extremely demanding due to the requirement of basis functions of high angular momenta. The way out of these conceptual and computational difficulties is to explicitly build in the magnetic balance (MB) condition between the small and large components of the Dirac bispinors. However, a successful formulation that captures naturally the `missing' diamagnetism and meanwhile is free of numerical instabilities has not been achieved until 2007[24]. Now it is clear that there exist many equivalent ways[25,26] to incorporate the MB condition, in conjunction with a proper treatment of the distributed gauge origins[27]. For more details, we refer the reader to the comprehensive reviews[14,28].

Albeit a physical observable, absolute NMR shieldings cannot be measured accurately. Instead, they are usually translated from the nuclear spin-rotation (NSR) coupling constants that can be determined accurately through hyperfine splittings of molecular rotational spectra. However, the mapping relationship[23] between NSR coupling constants and NMR shieldings holds only in the nonrelativistic limit. Therefore, the so-obtained “experimental NMR shielding” is nonrelativistic in nature. In other words, a fully relativistic experimental measurement is translated into a nonrelativistic value, which necessarily breaks down for heavy atoms (even for atoms like C to F bonded to light ligands, relativistic effects are already sizable, ca. 2–5 ppm). To establish a “relativistic mapping” between NSR and NMR, we have to (1) formulate a body-fixed relativistic molecular Hamiltonian for spectroscopies involving nuclear degrees of freedom, (2) formulate a rigorous theory of NSR coupling constants, and (3) find a connection between NSR coupling constants and NMR shieldings. All these have been achieved[29-31]. With this new relativistic mapping, that goes back to the nonrelativistic one in the limit of an infinite speed of light, new experimental shielding scales can be established[32].

It is believed that all the fundamentals pertinent to relativistic Hamiltonians, relativistic wave functions and relativistic properties have well been understood, such that the big picture of RMQM has been established. However, this does not imply that RMQM has come to an end. Rather, it implies that RMQM has entered a new era.

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New Research 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, Prof. of Experimental Physics/Solid State Physics, Ruhr-Univ. Bochum
2013 – 2018 Visiting Senior Research Professor, University of Mainz
since 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, 2013-2018.

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.

Professional activities:

Advisor and Co-advisor of 51 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);Member and Chair of the scientific councils at the Hahn-Meitner Institute Berlin, Institut Laue-Langevin, Grenoble, Materials Research Laboratory, University of Illinois at U – C.

Publications:

More than 500 refereed scientific publications in technical journals, 36 review papers and book chapters, editor of five books , author of the textbook "Physik" , Thieme publisher, 2nd edition 2016, Textbook "Medical Physics", de Gruyter publisher, 1st edition 2017.

Research activities:
Physical properties of hydrogen in metals; structure, dynamics, and magnetism of graphite intercalation compounds; strain state and strain relaxation in semiconductor heterostructures; order and disorder in metal superlattices and heterostructures; oxidation of epitaxial metal films; magnetic phase transitions in rare earth films and superlattices, phonons in layered compounds; magnetism of thin films and heterostructures; proximity effects between superconductors and ferromagnets; tuning of magnetism in spintronic materials; shear behavior of polymer chains; shear induced order of micellar polymer solutions; relaxation rates of polymer micelles; sliding and depletion lengths of Newtonian fluids at the solid-liquid interface; magnetic x-ray and neutron scattering, magneto-optics; magnetic nanostructures with spin-ice properties; magnetic nanoclusters, odd-triplett superconductivity; time-resolved magnetization precession and magnetization reversal processes, antiferromagnetic spintronics.
Teaching activities:
Introductory Physics Course; Modern Physics; Condensed Matter Physics; X-ray and neutron scattering; Exploring Condensed Matter at Large Scale Facilities; Physical Properties of Hydrogen in Metals; Condensed Matter Magnetism; Medical Physics. Numerous Lectures at National and International Summer Schools.

Selection of publications in 2020

Artificial Magnetic Pattern Arrays Probed by Polarized Neutron Reflectivity

Dmitry Gorkov, Boris P. Toperverg, and **Hartmut Zabel**
Nanomaterials **2020**, 10, 851; doi:10.3390/nano10050851

Abstract
Traditionally, neutron scattering is an essential method for the analysis of spin structures and spin excitations in bulk materials. Over the last 30 years, polarized neutron scattering in terms of reflectometry has also contributed largely to the analysis of magnetic thin films and magnetic multilayers. More recently it has been shown that polarized neutron reflectivity is, in addition, a suitable tool for the study of thin films laterally patterned with magnetic stripes or islands. We provide a brief overview of the fundamental properties of polarized neutron reflectivity, considering different domain states, domain fluctuations, and different domain sizes with respect to the neutron coherence volume. The discussion is exemplified by a set of simulated reflectivities assuming either complete polarization and polarization analysis, or a reduced form of polarized neutron reflectivity without polarization analysis. Furthermore, we emphasize the importance of the neutron coherence volume for the interpretation of specular and off-specular intensity maps, in particular when studying laterally non-homogeneous magnetic films. Finally, experimental results, fits, and simulations are shown for specular and off-specular scattering from a magnetic film that has been lithographically patterned into a periodic stripe array. These experiments demonstrate the different and mutually complementary information that can be gained when orienting the stripe array parallel or perpendicular to the scattering plane.

Introduction

Nanomagnetism is a key field for fundamental studies and technical applications of magnetic materials on the nanometer scale. In particular, in spintronics and magnonics, nanomagnetic systems are widely used as sensors, for logic circuits, and for data storage.

Nanomagnetic systems either consist of artificially arranged multilayers or laterally patterned islands, or a combination thereof. The artificial arrangements of various magnetic elements or compounds produces a rich environment for studying the effect of interfaces, symmetries, and interactions on their magnetic properties. Among the many methods that are used for analyzing the magnetism of artificial magnetic nanostructures, neutron scattering is less common but very powerful. Neutron scattering is more prominent for probing the magnetic properties of bulk materials. However, it can also be very useful as an analytical tool for studying magnetic nanostructures. The main aim of this contribution is a discussion of polarized neutron reflectivity (PNR) on on thin films patterned into a periodic array of micro-stripes. The scattering geometry for PNR is shown in Fig. 1.

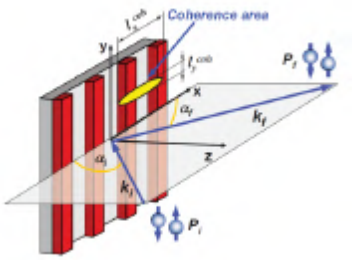

Fig. 1 - Sketch of the sample and beam geometry for polarized neutron reflectometry (PNR) experiments with one-dimensional polarization analysis along theY-axis. The elongated ellipsoid indicates the coherence volume of neutrons defined by the beam divergence and the wavelength spread. Here the ellipsoid is oriented parallel to the stripe array.

Probing interspatial magnetic flux distributions in ferromagnetic stripe arrays by specular and off-specular polarized neutron scattering

D. Gorkov, B. P. Toperverg, and **H. Zabel**
PHYSICAL REVIEW B **101**, 224404 (2020),
https://doi.org/10.1103/PhysRevB.101.224404

Abstract
Edge roughness in magnetic stripe arrays is an important structural parameter with a sizable impact on magnetic domains, domain correlation, pinning and propagation of domain walls in micro- and nanostripes proposed for data storage and logic devices. We have investigated two different stripe arrays fabricated by lithographic methods from permalloy Fe22Ni78, one with rough edges and another one with smooth edges. Performing polarized neutron reflectivity and polarized neutron off-specular scattering both patterns yield specular reflectivity curves with pronounced Kiessig fringes and well resolved Bragg bands in the off-specular regime due to the lateral periodicity. When applying a saturating magnetic field perpendicular to the stripes, a significant diffuse scattering can be detected close to the total reflection edge where it is enhanced by the Yoneda effect. This diffuse magnetic scattering can be attributed to inhomogeneities of the magnetic induction in the empty space between the stripes. In contrast, the sample with much less edge roughness does not exhibit off-specular diffuse scattering. Thus polarized neutron scattering from stripe patterns is a suitable tool for quantitative characterization of

inhomogeneous magnetic flux distribution in the interspace between magnetic stripes invoked by their edge roughness.

Introduction

Magnetic stripes or wires having a width on the micro- to nanometer length scale are important objects of research and development in the field of magnonics, magnetoelectronics, and spintronics. Nanowires with different aspect ratios confine magnetism to one dimension, providing a laboratory for investigations of magnetization reversal processes for controlling domain walls and determining domain wall velocities, for trapping skyrmions and for realization of various domain ground states. Furthermore, nanowires have been considered as building blocks for three-dimensional magnetic storage devices and for logic elements. As the size of the nanowires decreases, the fabrication of these wires with smooth edges becomes increasingly challenging. Edge roughness affects all characteristic magnetic properties of wires, including hysteresis and domain wall kinetics because of the trapping potential caused by edge roughness. Moreover, in arrays of nanowires edge roughness opens up a channel for interaction between the wires via stray magnetic flux emanating from rough edges. From a structural point of view, edge roughness can be characterized by a number of imaging techniques. However, determining quantitatively the magnetic flux between wires is more challenging. In this work, we show that polarized neutron scattering (PNS) techniques, combining specular polarized neutron reflectivity (PNR), Bragg diffraction as well as diffuse off-specular scattering (OSS), is a suitable method for characterizing the flux density in magnetic nanostripe arrays and in the interspace between the stripes. The design of the stripe array with edge roughness together with an image taken by scanning electron microscopy is shown in Fig. 2.

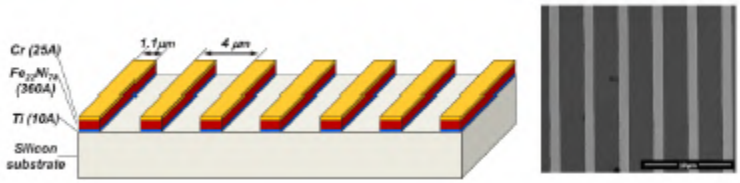

Fig. 2 - Scheme of the sample stack with nominal thicknesses of layers. (b) SEM images of the stripe array. Dark-grey color corresponds to the Si substrate.

Faster chiral versus collinear magnetic order recovery after optical excitation revealed by femtosecond XUV scattering

Nico Kerber, Dmitriy Ksenzov, Frank Freimuth, Flavio Capotondi, Emanuele Pedersoli, Ignacio Lopez-Quintas, Boris Seng, Joel Cramer, Kai Litzius, Daniel Lacour, **Hartmut Zabel**, Yuriy Mokrousov, Mathias Kläui & Christian Gutt

Nature communications (2020) 11:6304 | https://doi.org/10.1038/s41467-020-19613-z

Abstract

While chiral spin structures stabilized by Dzyaloshinskii-Moriya interaction (DMI) are candidates as novel information carriers, their dynamics on the fs-ps timescale is little

known. Since with the bulk Heisenberg exchange and the interfacial DMI two distinct exchange mechanisms are at play, the ultrafast dynamics of the chiral order needs to be ascertained and compared to the dynamics of the conventional collinear order. Using an XUV free electron laser we determine the fs-ps temporal evolution of the chiral order in domain walls in a magnetic thin film sample by an IR pump - X-ray magnetic scattering probe experiment. Upon demagnetization we observe that the dichroic (CL-CR) signal connected with the chiral order correlator $m_z m_x$ in the domain walls recovers significantly faster than the (CL + CR) sum signal representing the average collinear domain magnetization $m_z^2 + m_x^2$. We explore possible explanations based on spin structure dynamics and reduced transversal magnetization fluctuations inside the domain walls and find that the latter can explain the experimental data leading to different dynamics for collinear magnetic order and chiral magnetic order.

Introduction

In the field of magnetism and spintronics chiral magnetic structures, such as spin spirals, domain walls and skyrmions, are intensively investigated due to their fascinating properties. It has been shown that these structures are stabilized by the Dzyaloshinskii–Moriya interaction (DMI) that favors a chiral winding of the magnetization. This antisymmetric indirect exchange interaction requires materials with large spin–orbit coupling as well as a broken inversion symmetry, present in special bulk systems such as B20 compounds, or in interfacial systems such as heavy metal/ferromagnet multilayer stacks. The domain-wall type (Néel or Bloch) and chirality of the spin textures can be accessed in real space by imaging techniques, or in reciprocal space by (resonant) magnetic X ray scattering. The chiral wall spin structure is of key importance as it governs the dynamical properties of domain walls and skyrmions. Ultrafast pump-probe experiments have concentrated in the past on the collinear order in magnetic systems. In particular, as the ferromagnetic alignment minimizes the Heisenberg exchange energy, while the chiral order results from the DMI, the ultrafast dynamics of both orders needs to be probed individually. Moreover, since the characteristic timescale for the onset of the chiral magnetic order and its ultrafast dynamics are unexplored up to now, we need to ascertain both. The scattering geometry for this experiment is schematically shown in Fig. 3.

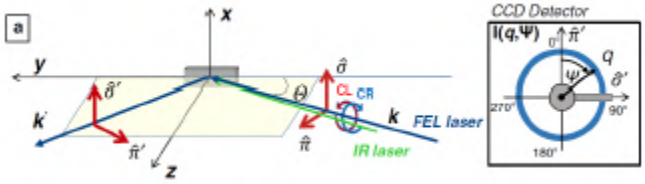

Fig. 3 – A magnetic thin film sample is pumped by an optical infrared laser pulse and probed by a circularly polarized X-ray laser pulse. A CCD detector records the azimuthal dependence of the magnetic small angle scattering pattern as function of time before and after pulsing.

Processes on Surfaces Related to Catalysis, the Structure & Dynamics of Water & Aqueous Solutions

by Anders Nilsson, Member EUAS

Short Biography

Current Work address

Division Chemical Physics, Department of Physics, AlbaNova University Center, Stockholm University, SE- 106 91Stockholm, Sweden

Field of research

X-ray Science, Surface Science, Heterogeneous Catalysis, Electrocatalysis, Photocatalysis, Structure and Dynamics of Water, Aqueous Solutions and Ultrafast Science.

Education and Professional Career:

1989 *Ph.D., Physics, Uppsala University, Uppsala, Sweden*
1989-92 *NFR Research Assistant, Dept. of Physics, Uppsala University, Sweden*
1993-99 *NFR Senior Researcher, Uppsala University, Sweden*
2000 *Professor in Physics, Uppsala University, Sweden*
2000-15 *Professor in Photon Science, Stanford University, USA*
2014- *Professor in Chemical Physics, Stockholm University, Sweden*
2020- *Recall Professor in Photon Science, Stanford University, USA*

Academic Achievements

Author and co-author of more than 300 scientific papers published in international refereed journals including Science, Nature, Nature Chemistry, Nature Communication, Physical Review Letters, Proceedings of the National Academy (US), Angewandte, Journal of American Chemical Society etc., one edited book and one non-scientific book, all of which are cited more than 30000 times and h-index 93 on Google Scholar (https://scholar.google.com/citations?hl=en&user=k4EfJAUAAAAJ&view_op=list_works&pagesize=100) or more than 23000 times and h-index 76 on ISI (ResearcherID: E-1943-2011). Participated in a large number of international conferences of which more than 170 as plenary, keynote or invited speaker. Have organized 6 summer schools, 2 international conferences, and 6 workshops. Have supervised or is supervising 10 Master-students and 35 PhD students and 30 post-doctoral researchers.

Science of water have received world-wide attention and was illustrated on the cover of Nature in 2014 and in 2004 Science Magazine selected it as one of the scientific breakthrough of the year. It has been reported in Swedish TV News (Rapport 23/12 2017), Washington Post, Le Monde, Daily Express, Die Speigel, La Republica and Dagens Nyheter. He participated in 2018 in the Nobel Dialogue about Water.

Recent Management Experience

2004-10 *Co-director for the Stanford Environmental Molecular Science Institute*
2007-10 *Deputy director for the Stanford Institute for Materials and Energy Science*
2008- *Director for the soft x-ray material program at Linac Coherent Light Source (LCLS), SLAC*
2010-13 *Chair of the Photon Science faculty, Stanford University*
2010-14 *Deputy director Center for Sustainable Energy through Catalysis (SUNCAT), Stanford University*
2012 *Co-organizer of a special symposium at the APS March meeting in Boston, Chemical Physics for New Energy*
2013 *Co-organizer of a special symposium at the APS March meeting in Baltimore, Recent Advances in Supercooled, Glassy and Nanoconfined Water*

2014 *Co-organizer of the Nordita Program, Water-the most anomalous liquid held October 13-November 7*
2014- *Member of the Scientific Advisory Committee for XFEL in Hamburg*
2015- *Organizer of the Soft X-ray Laser Effort for a Swedish FEL at MAXlab in Sweden*
2016- *Chair of the Condensed Matter, Atomic, Molecular and Optical Physics evaluation panel at the Swedish Research Council*
2017- *Chair of VR Committee for Inventory of Swedish Research Needs of X-ray Facilities.*

Awards &Honours

1994 *The Royal Oscars Award for Important Contributions in Science, Uppsala*
1998 *The Shirley Award for Excellent Research using Soft X-rays, Berkeley, USA*
2004 *Fellow of the Institute of Physics, London, UK*
2010 *Humboldt Senior Research Award, Germany*
2014 *Awarded Distinguished International Recruitment Grant from Swedish VR*
2015 *Awarded ERC Advanced Grant*
2015 *Honorary Doctorate, Danish Technical University*
2015 *Morino Lectureship Award, University of Tokyo, Japan*
2018 *Welch Foundation Lectureship Award, USA*

Achievements of Anders Nilsson

A central aspect of Nilsson's research work in chemical physics has been to investigate processes on surfaces related to catalysis and the structure and dynamics of water and aqueous solutions. He has taking these research topics to a new level by utilizing the capabilities of the new x-ray laser sources such as the Linac Coherent Light Source (LCLS) at SLAC National Accelerator Laboratory and other sources around the world. Let me here go through the recent breakthroughs in ultrafast dynamics in surface chemistry and fundamental water science related to the still not fully understood anomalous properties.

Nilsson has for several decades developed x-ray spectroscopies to probe the electronic structure and bonding of molecules on surfaces. Some of his early work has led to a revised picture of the surface chemical bond of importance for catalysis (Chemical Bonding on Surfaces and Interfaces, edited Nilsson, Pettersson and Nørskov, Elsevier, 2008.). He developed the "core hole clock method" that allows to follow ultrafast electron hopping or dissociation processes on time scales of the order of 100as-10fs (*Phys. Rev. Lett's.* **68**, 1892 (1992); **76**, 1380 (1996); **99** (2007) 217406). This methodology has been used to probe electron delocalization processes in adsorbed molecules on surfaces and between water molecules in the liquid phase.

With the building of LCLS, Nilsson had the vision that the x-ray spectroscopies he had been using to probe chemical bonding could be utilized to follow surface chemical reactions on ultrafast time scales using optical laser pump and soft x-ray probe techniques. He led a large collaboration to set up the first experiment to probe CO bond breaking on Ru (*Science* **339**, 1302 (2013)). He discovered the existence of the long-time proposed precursor state, a trapping state on the way towards desorption. The weakly adsorbed species appears roughly after a picosecond and could be identified from the x-ray spectroscopies to have almost gas phase character but there are some modifications due to the surface interaction that were detected in the spectroscopic process. The precursor state was further investigated recently in

more detail at the FERMI facility in Italy where there exists a more precise time synchronization between the x-ray and optical laser pulses (*PCCP*. **22**, 2677 (2020)) and it was shown that most of the molecules entering the weakly adsorbed state becomes readsorbed as the surface cools down.

Another major breakthrough at LCLS was the ultrafast probing of CO oxidation on Ru (*Science* **347**, 978 (2015)) where the transition state region was observed for the first time in a catalytic surface reaction. The experiment allowed a dismantlement of different times scales in the reaction after the optical pump. The adsorbed oxygen atom was activated to move from its strongly bonded hollow site position within 300 femtoseconds, the CO molecule started to move around 500 femtosecond and collisions between CO and O appeared in about 800 femtoseconds with molecules interacting with a spectroscopic signature of a weak elongated bond formed between CO and O. The observation of the transition state region in CO oxidation was selected by BES at DOE as one of the 10 top breakthroughs of the year 2015.

Using x-rays instead of optical lasers to initiate surface reactions it was recently shown upon selective excitation of electron states associated with the oxygen atom that CO_2 was primarily formed whereas exciting below the resonance or on the CO 2π^* resonance mostly CO desorption was detected (*J. Chem. Phys.* **149**, 234707 (2018)). Here we have the demonstration of steering selectivity in surface chemical physics by utilizing selective excitation.

The anomalous physical properties of water become dramatically enhanced upon supercooling below the freezing point. In particular, power-law fits of thermodynamic response functions such as compressibility and heat capacity appear to diverge towards a mysterious temperature (T_S) of about 228 K, which has ignited an ongoing debate about conflicting theoretical scenarios for the origin of this anomalous increase in entropy and volume fluctuations. However, water crystallization has prevented measurements of the bulk liquid phase below the homogeneous nucleation temperature (T_H) leading to a "no-man's land" devoid of experimental results regarding the structure of the liquid and response functions. Nilsson recently demonstrated a new experimental approach to study the structure of liquid states into the supercooled regime below T_H based on the use of femtosecond pulses generated by the LCLS x-ray laser to probe evaporatively cooled micron-sized droplets (*Nature* **510**, 381 (2014)). He could show that the water structure is continuous changing into a tetrahedral liquid without any phase transitions. He took the next step on probing the supercooled water droplets down to 227 K using small angle x-ray scattering at the x-ray laser PAL in Korea that allowed the determination of the isothermal compressibility and correlation length (*Science* **358**, 1589 (2017)). These response function diverged but not to infinity but instead to maxima at 229 K indicating the existence of a Widom line. Such a line corresponds to the extension of the phase transition line between two macroscopic liquid states beyond a critical point into the one phase region in the PT phase diagram. Thereby is the existence of a critical point in supercooled water a fully consistent explanation for the water's anomalous properties.

Nilsson has also used x-ray correlation spectroscopy techniques to access water

dynamics during a phase transition between high-density and low-density states that allowed the determination of diffusion coefficients (*PNAS* **114**, 8193 (2017)). The observation of diffusion demonstrated the existence of two macroscopic liquids in the ultraviscous region of water. This study was selected by Discover Magazine as one of the 100 top breakthroughs of the year 2017 in all scientific disciplines. This study was recently extended to higher temperatures using ultrafast heating of high-density state with an IR laser and then using the PAL x-ray laser to probe the liquid state during the decompression (*Science* **370**, 978 (2020)). Indeed, a low-density state appeared faster than ice crystallization demonstrating the existence of a liquid-liquid transition and further supporting the critical point hypothesis to explain the water anomalies. He also initiated the ability to probe ultrafast equilibrium dynamics in water using speckle visibility spectroscopy at LCLS indicating that even on 10 femtosecond timescales the hydrogen bonding network controls the motion and not ballistic dynamics (*Nature Comm.* **9**, 1917 (2018)).

Fifty Years of Bisphosphonates: What are their Mechanical Effects on Bone?

by David B. Burr, Member EUAS

Short Biography

David B. Burr
Distinguished Professor of Anatomy and Cell Biology, and Biomedical Engineering
Indiana University School of Medicine, and Indiana University-Purdue University Indianapolis (IUPUI)

Employment

1977-1978	*Instructor in Gross Anatomy, Department of Anatomy, University of Kansas Medical Center*
	Assistant Professor of Anatomy, Department of Anatomy, University of Kansas M Medical Center
1980-1983	*Assistant Professor of Anatomy and Orthopedic Surgery, Departments of Anatomy and Orthopedic Surgery, West Virginia University Medical School*
1983-1986	*Associate Professor of Anatomy and Orthopedic Surgery, Departments of Anatomy and Orthopedic Surgery, West Virginia University Medical School*
1986-1990	*Professor of Anatomy and Orthopedic Surgery, Departments of Anatomy and Orthopedic Surgery, West Virginia University Medical School*
1990-2010	*Professor and Chair of Anatomy and Cell Biology, Indiana University School of Medicine*
2011-2019	*Professor of Anatomy and Cell Biology, Indiana University School of Medicine*
1990-2009	*Professor of Orthopedic Surgery, Indiana University School of Medicine*
2000-2019	*Professor of Biomedical Engineering (IUPUI and Purdue University)*
	2012-2015 Non-Clinician Research Scientist, Richard Roudebush VA Medical Center, Indianapolis
2012-2018	*Associate Vice-Chancellor for Research, IUPUI*
2013-Present	*Distinguished Professor, Indiana University; Distinguished Professor Emeritus (2019-Present), with appointments in the Depts. of Anatomy, Cell Biology and Physiology (School of Medicine), and in Biomedical Engineering (IUPUI)*

Other Experience

2001	*President, Association of Anatomy, Cell Biology and Neurobiology Chairs*
2007-2009	*President, American Association of Anatomists*
2008-2009	*President, Orthopaedic Research Society*
2009-2013	*Delegate, General Assembly, International Federation of Associations of Anatomists*
2004-2013	*Associate Editor, Bone*
2013-present	*Editor, Bone*
2004-2019	*Associate Editor, Journal of Neuronal and Musculoskeletal Interactions*
2011	*Guest Editor (with R. Graham Russell) for Special Issue of BONE on Bisphosphonates*
2011-2013	*Section Editor (Skeletal Biology), Current Osteoporosis Reports*
2014-2020	*Editor-in-Chief, Current Osteoporosis Reports*
2014-2018	*Board of Directors, Federation of Associated Societies of Experimental Biology (FASEB)*
2015-2018	*Chair, Scientific Advisory Board, Fibrous Dysplasia Foundation (Member, 2020-Present)*
2019-2020	*Guest Editor (with P. Zaslansky and C. Fleck) for Special Issue of BONE in honor of John D. Currey*

2020-2021 Guest Editor (with Tamara Alliston and Elise Morgan) for Special Issue of BONE on Mechanobiology

Honors

1997 Honorary Chairman, 27th International Sun Valley Hard Tissue Workshop
2002 First Louis V. Avioli Best Article Award, Calcified Tissue International and Springer-Verlag (co-recipient with Jiliang Li and Tasuku Mashiba)
2008 Borelli Award, American Society of Biomechanics
2009 Fellow, American Association of Anatomists
2010 Chief Scientist Pro-Tempore, Hospital for Special Surgery
2010 Gideon A. Rodan Award for Excellence in Mentorship, American Society for Bone and Mineral Research (ASBMR)
2013 Named Distinguished Professor of Indiana University
2015 Henry Gray Scientific Award, American Association of Anatomists
2018 Fellow, Orthopaedic Research Society
2018 Albert Nelson Marquis Lifetime Achievement Award, Marquis Who's Who
2019 Fellow, American Society for Bone and Mineral Research
2019 Two Fellowship Awards for post-doctoral fellows, and one Leadership Award for faculty were named/endowed in my honor: David B. Burr Educational Fellowship; David B. Burr Musculoskeletal Fellowship; David B. Burr Service and Leadership Award (presented annually by the Indiana Center for Musculoskeletal Research)
2019 W.S.S. Jee Remodeling in Bone (RIB) Award, ORS Musculoskeletal Biology Workshop at Sun Valley
2020 Bicentennial Medal, awarded by Indiana University

I am an Indiana University Distinguished Professor Emeritus in the Department of Anatomy, Cell Biology, and Physiology, and Professor of Biomedical Engineering at IUPUI. I have 40 years of experience in studies involving histological and histomorphometric endpoints in both bone and cartilage. My primary area of research emphasis is to evaluate the effects of pharmacologic agents used to treat osteoporosis on bone matrix quality, specifically, the accumulation and repair of microdamage, changes in mineralization and alterations to the collagenous matrix. We have been investigating matrix effects of bisphosphonates and other anti-remodeling agents for many years using canine models. Since the early 1980's, I have studied the cross-talk between subchondral bone and cartilage deterioration, and still am frequently asked to talk about this in national and international venues. In the past several years, we have begun to investigate changes in matrix in Type 2 diabetes using similar approaches in the ZDSD and ZDF rat models of diabetes. My laboratory is equipped to characterize histological, immunohistochemical and dynamic histomorphometric features of different tissues, and to utilize bone density (BMD) and imaging techniques (μCT, pQCT) to analyze tissues in animal models. This has allowed me to bring both biological and mechanical concepts to the study of biological form, function and physiological processes at various length scales.

Fifty years of bisphosphonates: What are their mechanical effects on bone?

David B. Burr

Bone 138 (2020)

Abstract

After fifty years of experience with several generations of bisphosphonates (BPs), and 25 years after these drugs were approved for use in humans, their mechanical effects on bone

are still not fully understood. Certainly, these drugs have transformed the treatment of osteoporosis in both men and women. There is no question that they do prevent fractures related to low bone mass, and there is widespread agreement that they increase strength and stiffness of the vertebrae. There is less consensus, however, about their effects on cortical bone, or on bone tissue properties in either trabecular or cortical bone, or their effects with longer periods of treatment. The consensus of most studies, both those based on ovariectomized and intact animal models and on testing of human bone, is that long-term treatment and/or high doses with certain BPs make the bone tissue more brittle and less tough. This translates into reduced energy to fracture and potentially a shorter bone fatigue life. Many studies have been done, but Interpretation of the results of these studies is complicated by variations in which BP is used, the animal model used, dose, duration, and methods of testing. Duration effects and effects on impact properties of bone are gaps that should be filled with additional testing.

Voluntary Chronic Heavy Alcohol Consumption in Male Rhesus Macaques Suppresses Cancellous Bone Formation and Increases Bone Marrow Adiposity

Arianna M. Kahler-Quesada, Kathleen A. Grant, Nicole A. R. Walter, Natali Newman, Matthew R. Allen, David B. Burr, Adam J. Branscum, Gianni F. Maddalozzo, Russell T. Turner and Urszula T. Iwaniec

ALCOHOLISM: CLINICAL AND EXPERIMENTAL RESEARCH Vol. 43, No. 12 December 2019

Background

Chronic heavy alcohol consumption is an established risk factor for bone fracture, butcomorbidities associated with alcohol intake may contribute to increased fracture rates in alcohol abusers. To address the specific effects of alcohol on bone, we used a nonhuman primate model and evaluated voluntary alcohol consumption on: (i) global markers of bone turnover in blood and (ii) cancellous bone mass, density, microarchitecture, turnover, and microdamage in lumbar vertebra.

Methods

Following a 4-month induction period, 6-year-old male rhesus macaques (Macaca mulatta, n = 13) voluntarily self-administered water or ethanol (EtOH; 4% w/v) for 22 h/d, 7 d/wk, for a total of 12 months. Control animals (n = 9) consumed an isocaloric maltose–dextrin solution. Tetracycline hydrochloride was administered orally 17 and 3 days prior to sacrifice to label mineralizing bone surfaces. Global skeletal response to EtOH was evaluated by measuring plasma osteocalcin and carboxyterminal collagen cross-links (CTX). Local response was evaluated in lumbar vertebra using dualenergy X-ray absorptiometry, microcomputed tomography, static and dynamic histomorphometry, and histological assessment of microdamage.

Results

Monkeys in the EtOH group consumed an average of 2.8 _ 0.2 (mean _ SE) g/kg/d of EtOH(30 _ 2%of total calories), resulting in an average blood EtOHconcentration of 88.3 _ 8.8 mg/dl 7 hours after the session onset. Plasma CTX and osteocalcin tended to be lower in EtOH-consuming monkeys compared to controls. Significant differences in bone mineral density in lumbar vertebrae 1 to 4 were not detected with treatment. However, cancellous bone volume fraction (in cores biopsied from the central region of the third vertebral body) was lower in EtOH-consuming monkeys compared to controls. Furthermore, EtOH-consumingmonkeys had lower osteoblast perimeter and mineralizing perimeter, no significant difference in osteoclast perimeter, and higher bone marrow adiposity than controls. No significant differences between groups were detected in microcrack density (2nd lumbar vertebra).

Conclusions

Voluntary chronic heavy EtOH consumption reduces cancellous bone formation in lumbar vertebra by decreasing osteoblast-lined bone perimeter, a response associated with an increase in bone marrow adiposity.

Skeletal Protection and Promotion of Microbiome Diversity by Dietary Boosting of the Endogenous Antioxidant Response

AmyY. Sato, Gretel G. Pellegrini, Meloney Cregor, Kevin McAndrews, Roy B. Choi, Maria Maiz, Olivia Johnson, Linda D. McCabe, George P. McCabe, Mario G. Ferruzzi, Mary A. Lila, Munro Peacock, David B. Burr, Cindy H. Nakatsu, Connie M. Weaver and Teresita Bellido

Journal of Bone and Mineral Research, 2020

Abstract

There is an unmet need for interventions with better compliance that prevent the adverse effects of sex steroid deficiency on the musculoskeletal system. We identified a blueberry cultivar (Montgomerym [Mont]) that added to the diet protects female mice from musculoskeletal loss and body weight changes induced by ovariectomy. Mont, but not other blueberries, increased the endogenous antioxidant response by bypassing the traditional antioxidant transcription factor Nrf2 and without activating estrogen receptor canonical signaling. Remarkably, Mont did not protect the male skeleton from androgen-induced bone loss. Moreover, Mont increased the variety of bacterial communities in the gut microbiome (α-diversity) more in female than in male mice; shifted the phylogenetic relatedness of bacterial communities (β-diversity) further in females than males; and increased the prevalence of the taxon Ruminococcus1 in females but not males. Therefore, this nonpharmacologic intervention (i) protects from estrogen but not androgen deficiency; (ii) preserves bone, skeletal muscle, and body composition; (iii) elicits antioxidant defense responses independently of classical antioxidant/estrogenic signaling; and (iv) increases gut microbiome diversity toward a healthier signature. These findings highlight the impact of nutrition on musculoskeletal and gut microbiome homeostasis and support the precision medicine principle of tailoring dietary interventions to patient individualities, like sex. © 2020 American Society for Bone and Mineral Research (ASBMR).

Photon Generation by Electron Transfer Reactions at Electrodes and the World Nanosensor Materials

by Kalathur Santhanam, Member EUAS

Short Biography

Kalathur S.V. Santhanam was born in Tirupati and obtained Bachelor of Science degree with Honors in first class in all the three subjects Chemistry, Physics and Mathematics at Sri Venkateswara University and did his doctoral degree under the supervision of Dr. V. R. Krishnan, Ph.D (Kansas) at the same University under University Grants Commission Scholarship and National Institute of Sciences of India fellowship. His thesis on controlled potential electrolysis was awarded the best doctoral thesis of the year by the University. Following the completion of the doctoral degree, he was awarded Welch Fellowship to do post-doctoral work at University of Texas at Austin (USA) with world famous Dr. Allen J. Bard, Ph.D (Harvard). He pioneered the field of electrogenerated chemiluminescence and organic electrochemistry. Following the completion of post-doctoral work, he moved to Tata Institute of Fundamental Research, Mumbai where he rose to the highest position as Senior Professor. He initiated studies on carbon nanotube electrode for bioelectrochemical studies, electrobioluminescence and organic conducting polymers. During this period, he was involved in collaboration with laser interferometry (with Dr. R.N. O'Brien, Ph.D (Manchester), University of Victoria, BC), bioelectrochemistry (with Dr. P.J. Elving, Ph.D (Princeton), University of Michigan, Ann Arbor, USA), University of Guelph, Canada, conducting polymer batteries (with Dr. O. Haas, PSI, Switzerland) and Brookhaven National Laboratory, USA. He joined Rochester Institute of Technology in 1998 where after serving for more than ten years as Director of Center for Materials Science and Engineering, is currently Professor in the School of Chemistry and Materials Science. He is an elected member of SAXON Academy of Sciences (Germany) and European Union Academy of Sciences. He is a life member of society for advancement of electrochemical science and technology (SAEST) and Bioelectrochemical Society of India. He is a member of number of other scientific societies.

Positions Present and Past

2012-Present	*Professor of Chemistry , Rochester Institute of Technology, Rochester, NY*
2002-2012	*Director of Materials Science and Engineering, and Professor of Chemistry, Rochester Institute of Technology, Rochester, NY, USA*
2000-2002	*Visiting Professor of Chemistry, Rochester Institute of Technology, Rochester, NY, USA*
1998-2000	*Consultant, Pactiv Corporation and adjunct professor at Rochester Institute of Technology, Rochester, NY, USA*
1993-1998	*Senior Professor, Tata Institute of Fundamental Research (TIFR), India*
1990-1993	*Professor, Tata Institute of Fundamental Research (TIFR), India*
1982-1990	*Associate Professor, Tata Institute of Fundamental Research (TIFR), Mumbai, India*
1976-1982	*Reader, Tata Institute of Fundamental Research (TIFR), Mumbai, India*
1969-1976	*Fellow, Tata Institute of Fundamental Research (TIFR), Mumbai, India*
1968-1969	*Visiting Fellow, Tata Institute of Fundamental Research (TIFR), Mumbai, India*
1967-1968	*University of Victoria, B.C., Canada*
1964-1967	*Welch Post-doctoral Fellow, University of Texas, Austin, Tx, USA*
1963-1964	*National Institute of Sciences of India (currently called Indian National Science Academy) Fellow, Sri Venkateswara University, Tirupati, India*
1960-1963	*University Grants Commission Scholar (UGC, New Delhi), Sri Venkateswara University, Tirupati, India*
1958-1960	*Demonstrator, Department of Technology, University of Madras, Madras, India*

Education

B.Sc (Hons)	*Major: Chemistry (First Class), Subsidiaries: Physics (First Class), Mathematics (First class)*

	Sri Venkateswara University, Tirupati, India
Ph.D.	*Thesis: Controlled Potential Coulometric Oxidation of Organic Compounds, Sri. Venkateswara University, Tirupati, India*
	Work done under University Grants Commission Scholarship and National Institute of Sciences of India Fellowship.
	Awarded the Best thesis of the Year.

Visiting Positions

1971-1973	*Visiting Scientist, University of Michigan, Ann Arbor, MI, USA*
1976	*Research Associate, University of Texas, Austin, TX, USA*
1979-1980	*Visiting Professor, University of Guelph, Ontario, Canada*
1980-1981	*University of Texas, Austin, TX, USA*
1982-1989	*Visiting Scientist, University of Victoria, B.C., Canada*
1986	*Visiting Scientist, Brookhaven National Laboratory, USA*
1989	*Visiting Scientist, CNRS, Meudon, France*
1989	*Visiting Fellowship, British Council, Mumbai, India*
1991-1992	*Visiting Scientist, Paul Scherrer Institute, Switzerland*
1998	*Visiting Scholar, Rensselaer Polytechnic Institute, Troy, USA*

Professional and Academic Honors

Chairman, Bombay Association for Science Education (1981-'84)
Chairman, Society for Advancement of Electrochemical Science & Technology SAEST (Bombay) (1985-'92)
Member, Scientific Advisory Committee of Central Electrochemical Research Institute (1975-'76)
Member, Scientific Committee of Nehru Science Center (1983-'86)
Member, Asian Coordinating Group of Chemistry X, UNESCO, New Delhi (15-16 February, 1993)
Chairman, Bioelectrochemical Society of India (1990-1998)
Elected Full Member Sigma XI - The Scientific Honor Society of North America (1964)
Merit Certificate - Chemical Abstracts (1971)
Member Editorial board - Trans. SAEST, India (1973 -1984)
Recognized guide for Ph.D. degree- Bombay University, India (1984)
Member Editorial Board - Journal of Electro-Analytical Chemistry Bioelectrochemistry-Bioenergetics (1990 - 2002)
Invited speaker for Conducting polymer Energy Storage Systems-American Chemical Society Meeting, Washington D.C. (1992)
Prof. T.L. Rama Char Endowment Lecture - Electrochemical Society of India (1993)
Elected Corresponding Member of German Academy of Sciences - Sachsische Akademie der Wissenchaften (1995)
Golden Jubilee Fellow - UDCT, Bombay University (1995)
ABI Recognition Honorary Research Board of Advisors (2002)
Invitation to attend NSF-3-D Nanomanufacturing Workshop (2002)
Session Chairman-International workshop on Fuel Cell Technology for Advanced Vehicles, RIT (2002)
Chair the Carbon nanotubes session at the 203rd Electrochemical Society Meeting in Paris (2003)
Invited speaker in International Conference on Electroactive polymers (2007)
Certificate of Accomplishment by Commission for promoting pluralism (2007)
Honorable mention of Who is Who in USA (2008)
Invited speaker at Nanotube session of Electrochemical Society, Vancouver (2009)
Honorary member, Institute of Integrative Omics and Applied Biotechnology (IIOAB) (2009)
Certificate of appreciation for valuable contribution and dedicated service by American Chemical Society (2011)
Editor, Special issue, MDPI Journal Chemical Engineering (2018-2020)
Elected Member European Union Academy of Sciences (2020)

PUBLICATIONS

More than 200 papers in international journals

BOOKS PUBLISHED

Workshop on Electrochemical Instrumentation, SAEST(Bombay), 1985
(Co-authors: R. Sundaresan, M.K. Totlani)
Photoelectrochemical Solar Cells, Elsevier Science Publishers, Amsterdam, 1988 (co-, author: M. Sharon)
Ion-sensing Electrodes and Electrochemical Instrumentation, World
Scientific Publishers, Singapore-New Jersey- London, 1990 (Dedicated to my mentor Prof. A.J. Bard)
Metallic Corrosion (Co-editors: A.S. Khanna, S.N. Malhotra and M.K. Totlani); Wiley-Eastern, New Delhi, 1994
Introduction to Hydrogen Technology (co-authored: R. Press, A. Bailey,M.Miri and J. Takacs)
Wiley, NJ, 2009
Clean Energy: Hydrogen/Fuel cells Laboratory Manual, (co-authored: R. Press, A. Bailey, M.Miri and J. Takacs), World Scientific, Singapore, New Jersey, 2016
Introduction to Hydrogen Technology (co-authored: R. Press, A. Bailey, M.Miri and J. Takacs)
Wiley, NJ, 2017 (second edition)

Research

I started my research career at the University of Madras (now called Chennai) in Controlled potential electrolysis but had to move to Sri Venkateswara University when I was awarded the University Grants Commission Scholarship (UGC, New Delhi) to pursue this research under Dr. V.R. Krishnan, Ph.D. (Kansas). My interest grew in electrochemistry due to two distinguished scientists, Prof. A.N. Frumkin (Russian electrochemist, a nominee for Nobel Prize) and Prof. A.J. Bard (University Texas). When I presented my first paper on controlled potential oxidation of thiourea under the Chairmanship of Prof. Frumkin at Central Electrochemical Research Institute, he commented that it was a nice work. Later, this paper was published in Zeichrift fur physicalishe chemie [Zeitschrift fur Physikalische. Chemie (NF), 34, 312 (1962)] followed by another publication in American Chemical Society Journal [Anal. Chem., 33, 1493 (1961)]. Prof. Bard inspired me by his Analytical Chemistry Annual Reviews on Coulometry which led me to have an ambition to do post-doctoral research with him. I succeeded in getting an opportunity when I completed my Ph.D. degree. At that time, organic electrochemistry was a hot area as techniques like electron spin resonance (ESR) were used to trap the intermediates in the mechanism of the ultimate formation of the products. We were interested in the generation of free radicals of aromatic hydrocarbons like diphenyl anthracenes and examining the possibility of the free radical anion and free radical cation to react to produce the excited state of the molecule that would result in the emission of photons. We succeeded electrochemically by pulsing experiments and ESR identifications in evolving a mechanism for the emission [J. Am. Chem. Soc., 87, 139 (1965), J. Am.Chem. Soc., 88, 2669 (1966); J. Phys. Chem.,70, 404 (1966); J. Phys. Chem., 71, 2223 (1967)]. While the general mechanism envisages that the free radical anion and free radical cation of the same hydrocarbon will have enough energy to produce the first excited singlet state of the molecule, energetically deficient reactions were also identified to produce the excited state through the triplet state of the molecule. To distinguish the two routes of formation of the excited state, efficiency measurements and magnetic field effects were explored [J. Chem. Phys., 58, 821 (1973); Proc.Ind. Acad., 80A, 194 (1974); Can. J. Chem., 53, 76 (1975); Pramana, 5, 339 (1975); Chem. Phys. Lett., 51, 442 (1977); J. Chem. Soc. Chem. Commun., 2409 (1994); Chem. Phys., 185, 113 (1994)]. A direct generation of emission of photons was discovered during electrolysis of a heterocycle, carbazole; this does not require a pulsing technique to be used [Fluorescence, Ed. G.G.Guilabault, Chapter 14, MarcelDekker, New York, 1967; Canadian Journal of Chemistry, 47(8),1355-1359, 1969; Can. J. Chem., 49, 3577 (1971)].

From the above studies involving artificial systems, I turned to examine the processes that result in the emission of photons in real systems such as earthworms and fireflies. There are several genera of earthworms but out of which only a few of them produce photons. Lampito Maurutii is a species that produce photons upon excitation. I had the opportunity to do initial work on the electrochemistry of biological molecules at the University of Michigan, Ann Arbor [, J. Am. Chem. Soc., 95, 5482 (1973); Bio electro chem. Bioenergetics, J. Electroanal., (2), 147 (1974); J. Electrochem. Soc., 121, 345 (1974); J. Am. Chem. Soc., 96, 1653 (1974); J. Electrochem. Soc., 121,1032 (1974); J. Am. Chem. Soc., 97, 5083 (1975); J. Am. Chem. Soc., 97, 2591 (1975)]. To understand the mechanism of living systems producing photons, electrochemical techniques, electroporation and incorporation of the isolated active center into a nonbioluminescent earthworm have been examined and accomplished [J. Electroanal. Bioelectrochem. Bioenergetics, 192(14), 405 (1985); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 211 (15), 341 (1986); Proc. Ind. Acad. Sci., 97, 479 (1986); J. Electroanal. Chem. Biolectrochem. Bioenergetics, 213(17), 105 (1987); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 253(19), 9 (1988); J. Electroanl. Chem. Biolectrochem. Bioenergetics, 253(19), 21 (1988); J. Biolectrochem., 32, 211 (1993); Charge transfer effect on coelomic cells in exalted bioluminescence of Lampito mauritii in "Charge and Field effects in Bio-system-3, Eds. M.J. Allen et al, Birkhauser Pub., Boston, p.169 (1992); Bioelectrochemistry and Bioenergetics; 43, 197 (1997)]. We introduced electrochemiluminescence and electrobioluminescence as a tool for analytical determinations [Ind. J. Phys., 51B, 446 (1977); J. Electroanl. Chem. Biolectrochem. Bioenergetics, 276(22),219 (1989); J. Electroanal. Chem. Bioelectrochem. Bioenergetics, 276(22),231 (1989); J. Biolectrochem. Bioenergetics, 40,59 (1996)].

Organic Conducting Polymers

Discovery of polycarbazole which is formed during electrochemiluminescence on the anode led to investigation of its properties [J. Power sources, 32, 1 (1990); J. Mater. Chem. (Royal Society of Chemistry, London), 2(9), 965 (1992); Synthetic metals, 28, 27 (1989); Mol Crystals & Liquid Crystals, 160, 103 (1988); J. Solid state Electrochem., 2, 123 (1998); J. Solid state Electrochem., 2, 99 (1998); J. Pure and Applied Chemistry (IUPAC), 70, 1260 (1998); Macro '98, 395 (1998); Advanced Mater., 11, 1028 (1999)]. The developments in this area of activity led to construction of cotton fiber batteries and polycarbazole battery [Trends in Polymer Sci., 1, 284 (1993); Chem. Rev., 97, 207 (1997)].

Carbon Nanotubes and Graphene

The discovery of carbon nanotube opened up the possibility of its practical applications. We developed carbon nanotube electrode and demonstrated its potentiality for fast electron transfer reactions [J. Bioelectrochem. Bioenergetics, 41, 121 (1996); Advanced Mater., 11, 154 (1999); Nano Letters, 1, 77 (2001)]. Introduced nanodimensional reactions using carbon nanotubes [Int. J. Nanoscience, 1, 285, (2002); Int. J. Nanoscience, 1. 277, (2002); Fullerenes--Volume 13: Fullerenes and Nanotubes, 285-288 (2003); J. Nanosci. Nanotechnol. 14, 2679-2682 (2014); J. Nanosci. Nanotechnol. 14, 2842-2851 (2014)] and sensors [Sensors and Actuators, B: Chemical B106(2), 766-771 (2005), J. Nanoscience and nanotechnology**,** 8, 1 (2008); Sensors and Actuators B 142, 147–151 (2009); Encyclopedia of Nanoscience and Nanotechnology, Vo. 24, p.249, (2011); J. Nanoscience and nanotechnology, 10,3799 (2010); J. Nanoscience and nanotechnology, 10,3799 (2010); Sensors and Actuators B 191, 545– 552 (2014)]. Graphene as a 2D material provided an opportunity for its usage as an electrode for sensor and thermal applications. We developed a new electrochemical method of making graphene and graphene quantum dots that could be used without the need for purification and applied it to sensors and thermal applications [Patent No. US 9,840,782 B2, December 12, 2017; MRS Volume 3, Issue 22 (Energy and Sustainability), pp. 1221-1228 (2018); MRS Advances 3,15-16 (2018): 825-830; Journal of The Electrochemical Society, 165, 5, B232-B239 (2018):. Journal of The Electrochemical Society, 163, 166 (2016); Journal of Power Sources, 332, 337-344 (2016); Journal of The Electrochemical Society, 163 (6),E166-E172 (2016); MDPI *Chemical Engineering* 3. 80 (2019)]. Currently, efforts are being made to develop greenhouse gas sensors and nanopipette electrodes with graphene to achieve higher resolutions.

Recent publications

Electrochemical Approaches Towards sensing of viruses: A mini review

K.S.V. Santhanam**, Medical Devices and Sensors (Wiley),** 2020;00:e10148, DOI:10.1002/mds3.10148

This mini review focusses the development of electrochemical sensors for a variety of viruses, for example, West Nile virus, dengue (DENV-2, DENV-3, DENV-4), human phenotypes, H5N1, human norovirus, Japanese encephalitis (JEV), diarrhoea virus and rotavirus. These sensors are classified into four types based on Faradaic current measurement, impedance, conductivity and the current flow in a field effect transistor. While the first two have been well investigated, the latter two albeit in preliminary stages show great promise. Their simplicity,

precision, sensitivity and rapid analysis make them valuable over conventional methods. The Middle East respiratory syndrome coronavirus (MERS-CoV) can be assayed in 20 min with detection limit of 1 pg/ ml. The combination of biology with chemistry and material science could be utilized to develop disposable sensors for the rapid detection of SARS-CoV-2, a virus that has caused havoc around the globe.

Electrodeposition from a Graphene Bath: A Sustainable Copper Composite Alloy in a Graphene Matrix

Hayley Richardson,Charles Bopp,Bao Ha,Reeba Thomas and Kalathur S.V. Santhanam

J. Compos. Sci. 2021, 5(1), 9; https://doi.org/10.3390/jcs5010009

The leaching effect of metals has led to the introduction of government regulations for the safety of the environment and humans. This has led to the search for new alloys with long-lasting sustainability. Herein, we wish to report a new brass alloy containing carbon with a remarkable sustainability produced by electrodeposition from a graphene quantum dots bath. The electrochemical measurements were carried out using cyclic voltammetry, potentiodynamic analysis, and Tafel measurements, and the deposits were characterized by X-ray fluorescence spectroscopy (XRF), Raman imaging, X-ray diffraction (XRD), atomic force microscopy (AFM), and scanning electron microscopy (SEM) to understand the surface morphology and elemental compositions. The current–time transients in the potential-step electrolysis were used to investigate the nucleation and growth mechanism. The smooth and compact deposit obtained at −0.60 V showed a composition of Cu = 24.33 wt %; Zn = 0.089 wt %; and C = 75.57 wt %. The SEM and energy dispersion X-ray analysis revealed a surface morphology with a uniform distribution of the particles and the presence of Cu, Zn, and C. The corrosion density of the material is very much lower than that of conventional brass, suggesting a higher sustainability.

Interfacial Detection with Nanotube Pipette Laden Graphene Quantum Dots Electrode

H. Richardson, N.N.N. Ahamed, C. Bopp, R. Thomas and K.S.V. Santhanam*, MRS Advances (2021)

Single cell analysis is an emerging technology that can provide a mechanistic understanding of complex biological systems and cell heterogeneity. Any disruption of its activity can be monitored through interfacial bioelectrochemistry. A new glass nanopipette electrode laden with graphene quantum dots (20-50 nm) has been constructed for in vitro interfacial bio-electrochemical studies. A platinum or copper wire (0.0006” dia) was placed inside the glass nano pipette with a tip size of 1 mm which was subsequently covered with graphene by dip coating. The glass nanopipette has been characterized by X-ray fluorescence as containing Si (96.82%), K (2.65%) and Fe (0.20%). The suitability of the electrode for studies involving oxidative stress produced by p-aminophenol (PAP) that results in membrane disruption and the frequency of molecular attachment of PAP to graphene has been relevant to the understanding of cell disruption. In this context, the electrochemical oxidation of PAP has been probed in vitro through differential pulse voltammetry (DPV) using the glass nanopipette electrode. The new electrode shows promise for examining electroactive neurotransmitter during its functioning in chronic diseases.

Deeper Understanding of the Mechanisms of Human Cancers and New Targets for Cancer Therapeutics

by Carlos Cordon-Cardo, Member EUAS

Short Biography

EDUCATION

1972 - 1975	*B.S. - Biology - "Santa Ana" College, Mataro, Spain.*
1980	*M.D. - Autonomous University of Barcelona, School of Medicine, Barcelona.*
1985	*Ph.D. - Cornell University Medical College, Graduate School of Medical Sciences, New York. Ph.D. in Cell Biology and Genetics.*
1982 - 1983	*Research Fellow, Department of Pathology, MSKCC, New York.*
1983 - 1987	*Special Fellow, Immunopathology, Department of Pathology, MSKCC.*

LICENSURE

1981	*M.D. License - Madrid, Spain.*
2016 - Present	*NYSDOH – Certificate of Qualification as Laboratory Director.*

NYSDOH – Certificate of Qualification (CQ Code: CORDC1). Dr. Cordon-Cardo is qualified to act as Laboratory Director in the following categories: Cytogenetics, Genetic Testing (limited to molecular pathology), Histocompatibility, Oncology, Molecular and Cellular Tumor Markers, Soluble Tumor Markers, Transplant Monitoring, Virology (limited to FDA-approved molecular tests and antigen detection assays).

HONORS/AWARDS

1985	*Academic Achievement - Graduate School of Medical Sciences Cornell University Medical College, New York, May 1985*
1986	*Catedratico Auxiliar "Ad Honorem," Universidad Central del Caribe School of Medicine, Puerto Rico*
1989	*The American Academy of Pediatrics, Honorable Mention Award - Urology Section, October 1989*
1991	*Louise and Alliston Boyer Young Investigator Award, Memorial Sloan-Kettering Cancer Center, New York, May 1991*
1994	*Paul Harris Award - Rotary International, Barcelona, December 1994*
1995	*Jaime Esperalba Award - Academia de Ciencias Mediques de Catalunya i Balears, June 1995*
1995	*Annual Scientific Award - Academia Medico-Quirurgica Española. "Academico de Numero" - Madrid, December 1995*
1996	*"Roll of Honour" - International Union Against Cancer (UICC), Geneva, Switzerland*
1996	*"C.G. Ahlstrom Lecture" and "Medal of the Swedish Society of Physicians" - Stockholm, Sweden, November 1996*
1999	*The Ramon y Cajal Lectures. The Spanish Institute, New York, February 1999*
2000	*"Don Santiago Ramon y Cajal Memorial Lecture," Spanish American Medical and Dental Society, New York, October 2000*
2002	*"Premio Europa 2002," La Rebotica, Madrid, Spain, June 2002*
2002	*"American Registry of Outstanding Professionals – Lifetime Member"*
2003	*President, Scientific Committee "I International Health Fair," Santiago de Compostela, Spain, March 2003*
2003	*"Key Note Lecture," 2nd International Conference on Translational Research and Pre-Clinical Strategies in Radiation Oncology, Lugano, Switzerland, March 2003*
2003	*Honorary Member, "Spanish American Medical and Dental Society." Delivered the "Don Santiago Ramon y Cajal Memorial Lecture," Spanish American Medical and Dental Society, New York, October 2003*
2003	*Member, Board of Directors, Queen Sofia Spanish Institute, New York, September 2003*
2003	*"16th Burchenal Lecture," 28th Annual Alumni Society Meeting, Memorial Sloan-Kettering, New York, November 2003*
2004	*"Key Note Lecture," Winter Meeting, Finnish Urological Association, Helsinki, Findland, February 2004*
2004	*Gold Medal – Scientific Merit, 125th Anniversary "Correo Gallego," Spain*

2004	*"Highly Cited Researcher – Clinical Medicine Category," Institute of Scientific Information (ISI) (http://www.isihighlycited.com)*
2004	*Gold Medal – Medical Sciences, Govierno de Galicia, Spain*
2005	*President, Scientific Committee "II International Health Fair," Santiago de Compostela, Spain, April 2005*
2005	*"Special Lecture," 20th European Congress of Pathology, Paris, France*
2006	*"Lliço Pi i Sunyer," Universidad de Barcelona, Spain*
2006	*"Gold Medal," Fundacion Clinica Ruber, Madrid, Spain*
2006	*"Doctor Honoris Causa," Universidad de Barcelona, Spain*
2007	*"Member of Honor," Reial Academia de Medicina de Catalunya, Spain*
2007	*"V Premio de Periodismo SEOM," with Dr. J. Corbella, Madrid, Spain*
2008	*Academic Endowed Chair: "Chernow Family Professor of Clinical Urological Sciences" - College of Physicians and Surgeons, Columbia University, New York.*
2009	*Special Lecture, "Accademia Lancisiana," Rome, Italy*
2009	*"Alon Dembo Visiting Professor Lecture," Toronto, Canada*
2009	*"Nobility in Science Award," The Sarcoma Foundation of America, New York*
2009	*"Cristóbal Gabarrón Prize for Science and Research," Valladolid, Spain*
2011	*Honorary Member, Societa Italiana di Urologia*
2012	*"Distinguished Alumnus Award" Weill-Cornell Graduate School of Medical Science, Cornell University.*
2013	*"Top Pathologist" Award, Leading Physicians of America*
2013	*First Saul Gusberg Memorial Lecture, Icahn School of Medicine at Mount Sinai*
2013	*Keynote Lecture, International Liver Cancer Association 2013 Annual Meeting*
2013	*"List of 400 Most Highly Influential Biomedical Researchers Worldwide," European Journal of Clinical Investigation*
2014	*Rod and Ceil Mortel Visiting Scholar in Cancer Research Lecture, Penn State College of Medicine*
2014	*Department of Pathology and Laboratory Medicine Annual Graduation Lecture, Rutgers Robert Wood Johnson Medical School*
2014	*"Thought Leader" Award, Agilent Technologies*
2015	*Keynote Lecture, Global Congress on Prostate Cancer (PROSCA15), Rome, Italy*
2015	*Special Lecture, Seminars in Genitourinary Oncology, Dana-Farber/Brigham and Women's Cancer Center, Boston, USA*
2015	*Keynote Lecture, American Association of Pathologists' Assistants, 41st Annual Continuing Education Conference, Toronto, Canada*
2015	*Keynote Lecture 7th European Multidisciplinary Meeting on Urological Cancers*
2015	*Keynote Lecture and Certificate of Honor, Museo de Historia de la Medicina y Ciencias de la Salud, University of Puerto Rico*
2016	*Special Lecture, Center for Cell Reprogramming, Georgetown University Medical Center*
2016	*Keynote Lecture XXXI Reunión Nacional del Grupo de Urología Oncológica, Spain*
2016	*Keynote Lecture Nordic Life Science Conference, Stockholm, Sweeden*
2016	*Special Lecture, Karolinska Institute, Stockholm, Seewen*
2016	*Keynote Lecture European School of Radiology, Lisbon, Portugal*
2017	*Member, Organizing Committee, Frontiers in Academic Pathology, New York*
2017	*President, Organizing Committee, 15th Meeting of The International Bladder Cancer Network, Lisbon, Portugal*
2017	*Fellow, Royal Society of Medicine, London, UK*
2018	*Member, Fundacion Gadea Ciencia, Spain*
2020	*Member, European Union Academy of Sciences (EUAS)*
2020	*"List of 500 Most Highly Cited Researchers Worldwide," Google Scholar*

Research Profile

Our basic and translational research studies in cancer assisted in laying the foundation, and later the implementation, of molecular pathology as an academic discipline. They have also aided to establish a deeper understanding of the mechanisms of tumor initiation and progression. Work from our group has generated clinical tangibles such as novel biomarkers for precise diagnosis and for highly accurate prediction, using innovatiove deep-learning and artificial intelligence (AI), and identified new targets for cancer therapeutics. Our laboratory is nationally and internationally renowned for its contributions to experimental pathology and molecular oncology, producing documented breakthroughs in the areas of multi-drug resistance, tumor suppression, and tumor suppressor gene-oncogene interactions. Groundbreaking research from our lab has produced novel insights into models for tumor

progression, such as defining two distinct pathways for early bladder cancer initiation; and evidence of the critical role of androgen receptor overexpression in the progression of prostate cancer. Expression profiling using genomics and computational biology approaches has been a logical extension of the work carried out in our lab, which in turn has provided insights into the molecular classification of certain human solid tumors, including bladder and prostate carcinomas, and soft tissue sarcomas. More recently, studies from our group have linked adult stem cells and cancer, and we have reported on the discovery of a subpopulation of human tumor initiating cells with stem properties. This new cancer stem cell has been identified in other solid tumors analyzed, including breast, lung and colon carcinomas.

Clinical Profile

Innovative applications in molecular medicine from our laboratory were among the first to be applied as clinical services. Work conducted with Drs. Old, Houghton and Cheung from MSKCC established some of the early monoclonal antibody targeted therapies, including anti-gangliosides GD3 and GD2 for melanoma and neuroblastoma. We also collaborated with Dr. Slamon in the characterization of anti-Her2/Neu antibodies, and early phases of Herceptin-based breast cancer treatments; and with Dr. Mendelsohn in the characterization and clinical application of anti-EGFR antibodies. Through the years we discovered and/or validated multiple biomarkers of clinical utility, such as antibodies to nephron-segment specific antigens (renal toxicity), cytokeratins (immunohistochemical reagents), and tumor-specific uroepthelial cells (cytology assessment of bladder cancer - FDA approved ImmunoCyt™). We were also involved in discovery and validation of genetic mutations for the early diagnosis of solid tumors. Several commercial products are based on our studies; including FDA approved UroVysion® (bladder cancer diagnosis). Our lab is considered one of the pioneers in molecular pathology, and the developer of "systems pathology." This is a new platform based on machine/deep learning AI approaches that generates novel algorithms obtained through the integration of phenotype and genotype of human diease tissue samples with the goal of optimizing treatment and improving outcome. Since my recruitment to Mount Sinai as Chairman of Pathology, I have recruited over fifty senior and junior faculty members, and have outlined a broad vision that redefines our discipline, placing it at the core of patient management and individualized medicine. I have also expanded biorepositories and databases to further strengthen translational research, enhancing our shared vision regarding personalized medicine.

Impact

I am and have been a Principal Investigator and Co-Investigator on multiple National Cancer Institute-funded grants, among other agencies, and have had uninterrupted peer-reviewed funding for over 30 years. I have lectured widely and am one of the most "Highly Cited Authors" by the Institute of Scientific Information in the biomedical sciences and one of the most "Highly Influential Biomedical Researchers" (1996-2011 – one of the top 400 over 15,153,100 author identifiers) by the European Society for Clinical Investigation. I published over 500 peer-reviewed articles, many in high impact journals such as Nature, Cell, Science, and their new affiliated journals, such as Nature Medicine, Nature Genetics and Cancer Cell (101,031 Citations; h-index 158 and i10-index 521 – as of 11/2020 per Google Scholar). Committed to educating the newest generation of scientists in my field, I have mentored over 70 investigators throughout their careers. I have received numerous awards in acknowledgement of my significant contributions to the field of pathology and molecular medicine, including among other the Boyer Young Investigator Award, the Gold Medal of the Swedish Society of Physicians, "Academico de Numero" of the Academia Medico-Quirurgica Española, and the

Distinguished Alumnus Award of Weill-Cornell Graduate School of Medical Science. I also received an honorary doctorate from the Universidad de Barcelona, and was named a Member of Honor at the Reial Academia de Medicina de Catalunya. I served as a member of the World Health Organization Collaborating Centers for Urologic Tumors, and the State Legislative Committee of the American Association for Cancer Research. I also served as the President for the Solid Tumor Chapter of the Association for Molecular Pathology, and Translational Chair for the Genitourinary Section of the Southwest Oncology Group. I also served as a member of the Review Committee for Cancer Centers and Research Programs of the NCI.

Dr. Carlos Cordon-Cardo earned his medical degree from the Autonomous University of Barcelona (1980), and his PhD in Cell Biology and Genetics from Cornell University (1985). Dr. Cordon-Cardo is Professor and Chair System-Wide of the Department of Pathology, Molecular and Cell-Based Medicine at the Icahn School of Medicine at Mount Sinai Health System. He was previously Professor and Vice-Chair of Pathology at Columbia University; and from 1987 to 2006 a faculty member in the Department of Pathology at Memorial Sloan-Kettering Cancer Center, where he created the Division of Molecular Pathology and served as its first Director; scaling the academic ranks from Assistant to Professor of Pathology at Weill Cornell Medical College, Cornell University. A pioneer of the oncologic molecular pathology discipline, Dr. Cordon-Cardo has helped establish a deeper understanding of the mechanisms of human cancers and new targets for cancer therapeutics, enhancing the vision of personalized medicine. His analyses of multi-drug resistance and alterations of tumor suppressor genes in human cancer have led to extraordinary breakthroughs in the way scientists understand and investigate the progression of certain solid-tumor cancers. More recently, studies from his laboratory have linked adult stem cells and cancer, reporting the discovery of a subpopulation of tumor initiating cells with stem properties which are also related to chemoresistance, immune-escape mechanism, and metastatic spread. He has developed and implemented a novel "systems pathology" platform, using artificial intelligence tools including deep-learning and novel algorithms, generating highly accurate mathematical models of cancer with the goal of optimizing treatment and improving patient outcome. During the present COVID-19 pandemic he designed and implemented a laboratory testing platform that includes qualitative and quantitative assays for viral SARS-CoV-2 detection and diagnosis, as well as qualitative and quantitative antibody testing for monitoring immunity and selection of antibody-rich convalescent individuals as potential plasma donors. The serology tests were given emergency use authorization (EUA) from both the New York State Department of Health (NYSDOH) and the FDA, as well as the CE-markering as an in vitro diagnostic device by the European Union. Under his leadership, over 100 autopsies of deceased COVID-19 patients were performed, being the largest series documented to date, and revealing novel pathophysiology stages of the disease. Dr. Cordon-Cardo is Principal Investigator on several National Cancer Institute grants, and has received uninterrupted NIH/NCI funding for the past 30 years. Dr. Cordon-Cardo has lectured widely and is one of the "Highly Cited Authors" by the Institute of Scientific Information, one of the "Highly Influential Biomedical Researchers" (one of the top 400 over 15,153,100 author identifiers) by the European Society for Clinical Investigation; and one of the top "List of 500 Most Highly Cited Researchers Worldwide," Google Scholar, Citations 101,185; h-index 158; i10-index 521 - as of 12/01/2020 (Google Scholar-2020). Dr. Cordon-Cardo holds 32 filed patents, including granted and pending, in the fields of medical diagnostics and therapeutics; and his work has been quoted in over 350,000 scholarly citations, including 8,069 patent citations (https://www.lens.org). Committed to educating the newest generation of scientists in his field, Dr. Cordon-Cardo has mentored over 70 investigators throughout his career. For this work and achievements Dr. Cordon-Cardo is the recipient of numerous honors and awards, including "Roll of Honour" of the International Union Against Cancer; Gold Medal of the Swedish Society of Physicians; Academico de Numero, Academia Medico-Quirurgica Española; Honorary Member, Spanish American Medical and Dental Society; Member of Honor, Reial Academia de Medicina de Catalunya; Doctor Honoris Causa, Universidad de Barcelona; Honorary Member, Societa Italiana di Urologia; Distinguished Alumnus Award, Weill-Cornell Graduate School of Medical Science, Cornell University; Fellow, Royal Society of Medicine, UK; and Member, European Union Academy of Sciences.

The Hygiene Hypothesis during a Pandemic: Consequences for the Human Microbiome

by B. Brett Finlay, Member EUAS

Short Biography

Dr. B. Brett Finlay is a Professor in the Michael Smith Laboratories, and the Departments of Biochemistry and Molecular Biology, and Microbiology and Immunology at the University of British Columbia. He obtained a B.Sc. (Honors) in Biochemistry at the University of Alberta, where he also did his Ph.D. (1986) in Biochemistry under Dr. William Paranchych, studying F-like plasmid conjugation. His post-doctoral studies were performed with Dr. Stanley Falkow at the Department of Medical Microbiology and Immunology at Stanford University School of Medicine, where he studied Salmonella invasion into host cells. In 1989, he joined UBC as an Assistant Professor in the Biotechnology Laboratory. Dr. Finlay's research interests are focussed on host-microbe interactions, at the molecular level. By combining cell biology with microbiology, he has been at the forefront of the field called Cellular Microbiology, making several fundamental discoveries in this area, and publishing over 525 papers (h index=140). His laboratory studies several pathogenic bacteria, including Salmonella and pathogenic E. coli, and more recently microbiota. He is well recognized internationally for his work, and has won several prestigious awards including the E.W.R. Steacie Prize, the CSM Fisher Scientific Award, CSM Roche Award, a MRC Scientist, five Howard Hughes International Research Scholar Awards, a CIHR Distinguished Investigator, BC Biotech Innovation Award, the Michael Smith Health Research Prize, the IDSA Squibb award, the Jacob Biely Prize, the prestigious Canadian Killam Health Sciences Prize, the Flavelle Medal of the Royal Society, the Queen Elizabeth II Diamond Jubilee Medal, the Prix Galien, is a Fellow of the Royal Society of Canada and the Canadian Academy of Health Sciences, is a Member of the German National Academy of Sciences, the European Union Academy of Sciences, the American Academy of Microbiology, Chair d'État, Collège de France and is the UBC Peter Wall Distinguished Professor. He is an Officer of the Order of Canada and Order of British Columbia, and inducted into the Canadian Medical Hall of Fame. He is a cofounder of Inimex Pharmaceuticals, Inc. and Microbiome Insights, scientific cofounder of Vedanta Pharmaceuticals and CommenSe, Director of the SARS Accelerated Vaccine Initiative, and Founding Director and Senior Fellow of CIFAR's Microbes and Humans. He is also the co-author of the books *Let Them Eat Dirt* and *The Whole Body Microbiome*.

The hygiene hypothesis during a pandemic: consequences for the human microbiome

B. Brett Finlay, Katherine R. Amato, Meghan Azad, Martin J. Blaser, Thomas C.G. Bosch, Huitung Chu, Maria Gloria Dominguez-Bello, Stanislav Dusko Ehrlich, Eran Elinav, Naama Geva-Zatorsky, Philippe Gros, Karen Guillemin, Frédéric Keck, Tal Korem, Margaret J. McFall-Ngai, Melissa K. Melby, Mark Nichter, Sven Pettersson, Hendrik Poinar, Tobias Rees, Carolina Tropini, Liping Zhao, Tamara Giles-Vernick

Abstract

The COVID-19 pandemic has the potential to affect the human microbiome in infected and uninfected individuals, having a substantial impact on human health over the long term. This pandemic intersects with a decades-long decline in microbial diversity and ancestral

microbes due to hygiene, antibiotics, and urban living (the hygiene hypothesis). High-risk groups succumbing to COVID-19 include those with pre-existing conditions, such as diabetes and obesity, which are also associated with microbiome abnormalities. Current pandemic control measures and practices will have broad, uneven, and potentially long-term effects for the human microbiome across the planet, given the implementation of physical separation, extensive hygiene, travel barriers and other measures that influence overall microbial loss and inability for re-inoculation. Although much remains uncertain or unknown about the virus and its consequences, implementing pandemic control practices could significantly affect the microbiome. In this Perspective, we explore many facets of COVID-19 induced societal changes and their possible effects on the microbiome, and discuss current and future challenges regarding the interplay between this pandemic and the microbiome. Recent recognition of the microbiome's influence on human health makes it critical to consider both how the microbiome, shaped by biosocial processes, affects susceptibility to the coronavirus, and conversely, how COVID-19 disease and prevention measures may affect the microbiome. This knowledge may prove key in prevention and treatment, and long-term biological and social outcomes of this pandemic.

Introduction

Humans are at a major crossroads of two major biosocial processes affecting the microbes that collectively inhabit us (our microbiome). The first process is the continued loss of gut microbial diversity and ancestral microbes among a large swath of the world's population. This loss of diversity has accelerated over the past several decades, likely affecting the co-existence between humans and our microbial residents and human health through the development of non-communicable diseases, including obesity, asthma, cardiovascular diseases, and brain diseases. The second process, the COVID-19 pandemic, is occurring at a breakneck pace across the planet, with diverse consequences for its populations. Large-scale pandemics entail widespread pathogen transfer between individuals, disruption of human activity, and they presumably affect microbial diversity and richness in infected and uninfected individuals. The interaction of these two processes is of critical importance for the collective human microbiome, and more broadly, for human health.

The model in the Figure outlines the process by which microbial diversity is lost. Gut microbial richness results from a balance of the acquisition and the loss of microbial species. The original hygiene hypothesis, first framed by David Strachan, has evolved into new, more complex and explicit hypotheses that capture many of the processes that influence gut microbial establishment and extinction. The most recent versions maintain that multiple changes among some of the world's populations have occasioned a loss of microbial diversity, which has accelerated over the last century because of many processes and practices: increased urbanization; overuse of antibiotics and other medications;, birth and infant feeding practices; intensified hygienic practices that disinfect bodies, homes and workplaces; reduced diversity in global diets (especially declining intake of dietary fiber and increased consumption of processed foods); and widespread use of tobacco, alcohol and other drugs.

Reduced acquisition and increased depletion of microbes over generations may lead to the extinction of microbial species ancestrally associated with humans; species may be permanently lost from the microbial pool unless re-inoculation from other sources occurs. First proposed by Blaser and independently by Rook, this longer-term loss is known as the disappearing microbiota hypothesis. Reduced microbial exposure resulting from diverse

social changes and associated increases in host inflammation have been linked to rising rates of chronic diseases, including obesity, diabetes, asthma, and various auto-immune diseases. Disruption of the microbiome pre-disposes us to multiple seemingly non-transmissible human diseases. Germfree animals, devoid of a microbiome, develop a high titer of IgE, the antibody isotype associated with allergic inflammation; loss of immune cells reacting to bacteria leads to severe allergic inflammation. In humans, exposure to rural environments and farm animals decreases the risk of allergy, whereas antibiotic consumption during early age is associated with an increased risk of developing allergic, autoimmune, and metabolic disease, presumably by affecting the balance of acquisition and loss of microbes. Notably, they may also heighten our susceptibility to infectious disease, just as climate change, deforestation, factory farms, and global connectivity intensify the likelihood of novel infectious disease pandemics.

This process of microbial diversity loss is occurring unevenly across the planet. Clean water, soap, and sanitation are not equally distributed to all people; access to and use of antibiotics, however, are widespread in low- and middle-income countries, constituting a "quick fix infrastructure," even for the poorest populations. Moreover, multiple vulnerable populations -- urban residents, racial and ethnic minorities, migrants, low-income earners – disproportionately suffer from certain chronic diseases linked to altered microbial functionality.

The COVID-19 pandemic itself is, of course, nested in a much longer history of pandemics that have afflicted humankind. From the Neolithic agricultural revolution, when larger human settlements facilitated the circulation of pathogens between humans and their domesticated animals, human history is punctuated with the repeated suffering of large epidemics and their disruptive consequences. Although notions of infection and practices of hygiene have varied across space and time, people have long used certain practices to manage pandemics – fleeing endemic areas, physical distancing, separating the sick from the healthy, and scapegoating of certain groups, often the most vulnerable to falling ill and dying. From the Black Death in the 14th century through smallpox epidemics in the 18th century, cholera in the 19th century, and the influenza pandemic of 1918-19, pandemics have weighed most heavily on the poor, migrants, and ethnic and racial minorities (19). As with past pandemics, COVID-19 mirrors and exacerbates existing inequalities, so that aging, poor, and chronically-ill populations suffer much higher morbidity and mortality.

The collision of the current pandemic with our decades-long process of hygienic and accompanying microbial changes, and the recent recognition of the importance of establishing and maintaining a healthy microbiome, provides a unique opportunity to explore in real time several key questions about humans and their microbiomes (Table). This moment can provoke investigation of how social inequalities, the human microbiome, and risk factors such as age or chronic disease affect susceptibility to the most serious outcomes of SARS-CoV-2 infection. It also allows examination of how COVID-19 control measures interact with various human practices and socioeconomic and ecological conditions that determine and modify microbial composition, the stability of these interrelations, and their capacity to establish or re-establish healthy microbial composition.

In this Perspective, we explore first what we know about the human microbiome's influence on COVID-19, and then examine in greater depth the current pandemic's potential effects on the human microbiome. We draw lessons from these intersecting processes and identify critical questions that should be tackled simultaneously by biomedical and social sciences researchers and public health actors for our near- and longer-term futures.

COVID-19 and the Microbiome

At this writing, we have little direct evidence of interactions between the human microbiome and SARS-CoV-2 infection. We do not know how the composition or metabolic activity of microbial populations living on mucosal surfaces (airway epithelial cells, gastrointestinal enterocytes) of the human body affect initial susceptibility to SARS-CoV-2 infection, subsequent pathogenesis, or outcome. Some intriguing observations, however, make this possibility difficult to ignore. Framing these unknown biological interactions are demographic and socio-economic factors – reflected in diet and other social determinants of health -- that render the elderly, racial and ethnic minorities, and those with lower socioeconomic status more likely to suffer worse outcomes to COVID-19 infection; these same groups have existing pathologies that correlate with dysbiosis of gut microbiota.

Recent studies in small groups of COVID-19 patients have identified major dysbiosis of the intestinal microbiome, with enrichment by opportunistic bacterial (Coprobacillus, Clostridium species) and fungal pathogens (Candida, Aspergilus species), and depletion of beneficial symbionts (Faecalibacterium) that are positively and inversely correlated with COVID-19 severity. In addition, an inverse correlation was noted between abundance of Bacteroides and SARS-Co-V2 load in fecal material during the course of hospitalization of these patients. Recently there have been reports of viable virus particles in the stool, although the significance and impact of these viral particles on the gut microbiome and infection transmission is not known. Recent demographic analyses of COVID-19-associated mortality rates (death/10^6) in 122 countries have suggested that inadequate sanitation and exposure to microbial diversity (including Gram-negative bacteria) may be associated with reduced COVID-19 associated mortality in developing and under-developed countries. The authors noted an inverse correlation between COVID-19 associated death rates and water quality scores, fraction of the population living in slums, and fraction with diarrhea. With these data, the authors proposed that microbially-stimulated, innately enhanced levels of type I interferon may be protective against COVID-19 mortality in these populations.

In addition to certain microbial taxa correlating with severity of Covid-19, several chronic conditions act as co-morbidity factors for COVID-19, including cardiovascular disease and associated hypertension, diabetes, obesity, and asthma. Among these conditions, obesity, type 2 diabetes and hypertension are the most important pre-disposing conditions for COVID-19 severe disease. Changes in the microbiome at times may modulate genetic susceptibility to these diseases in humans and animal models.

Recent data have shown that a major driver of the above-mentioned phenomena is the host immune system. The gut microbiome plays a major role in “training” the immune system, and changes in microbiome composition or activity may affect activity of several immune cell types (lymphoid, myeloid). These effects may be mediated in part by direct exposure of developing immune cells in situ in the gut, or by the production of different microbial metabolites that can act in other organs distant from the gut. COVID-19 fatalities are often associated with an overwhelming and pathological inflammatory response in the lungs, caused by over-production of pro-inflammatory cytokines (cytokine storm), as well as exhaustion of populations of immune cells ($CD8^+$ T cells). Interferons (IFNs) play an important role in the antiviral host response, which could be influenced by microbiome composition. Might differences in gut microbiome and associated immune cell programing influence individual host responses to SARS-CoV2 infection? Altering the microbiome composition through oral probiotics has been shown to alter the course and severity of

other respiratory infections, such as influenza.

Finally, SARS-CoV2 infection may directly affect the gut and airway microbiomes. The cell surface receptor for the virus (ACE2, angiotensin converting enzyme 2) is expressed on airway epithelial cells and on enterocytes along the digestive tract. Studies are underway to characterize the respiratory microbiome and COVID-19 infections. Although the data are limited, the probiotics *Lactobacillus* and *Bifidobacterium* appear depleted in the intestines of COVID-19 patients, indicating an abnormal state (termed dysbiosis). Moreover, hospitalized COVID-19 patients may receive high-dose antibiotics, which dramatically alters microbial populations. More detailed knowledge of microbiota changes during COVID-19 awaits further results.

Conclusion

The current pandemic has disrupted the world as we knew it. Despite the damage and turmoil that COVID-19 has already caused worldwide, it also reminds us the we live in a microbial world where microbes have a major impact on all facets of our existence. This pandemic presents a significant opportunity to study in real time the relationship between an infectious agent, the microbiome, precipitous and uneven social and economic changes, and their combined effects on health and disease. As we track changes in the microbiome during COVID-19, we can apply this knowledge to current pandemic control measures and recovery. These insights and new measures will provide a platform to improve our management of the next pandemic disruption.

Are non-communicable diseases communicable?

B.B Finlay, ***and*** CIFAR Humans and the Microbiome

The past century has seen a profound decrease in mortality rates across the world, accompanied by a marked shift from communicable diseases (caused by infectious microbes) to non-communicable diseases (NCDs) such as cardiovascular diseases, cancer, and respiratory diseases. NCDs account for more than 70% (41 million) of all deaths globally. NCDs are defined as diseases that are not transmissible directly from one person to another. The definition of NCDs rules out microbial involvement and instead focuses on other genetic, environmental and lifestyle factors. Increasing data show that: the microbiota is dysbiotic (altered) in individuals with various NCDs; in animal models of NCDs, transplantation of dysbiotic microbiota into healthy animals results in disease, and microbiota composition is shaped by close contact with others. Therefore, we propose that many NCDs may have a microbial component, and many NCDs may actually be to some extent communicable via the microbiota.

Infectious diseases are caused by the transmission of pathogens between individuals. However, the extent to which microbial dispersal between humans contributes to NCDs remains unclear. The human microbiota consists of the various microbes (including bacteria, fungi, viruses) living in and on the human body, and has a significant role in many physiological functions including digestion, immune system, and metabolic diseases. Although microbes reside on many body sites, the vast majority are in the gut, with bacteria being the best studied. Several examples of NCD transmission are found using animal models, but how transmissible is the human microbiota? Cohabitants and spouses have more similar gut bacterial microbiota than genetically similar siblings living separately. Microbiota are transmissible within both family and social networks, and spousal relationships can be

determined based on gut bacterial analysis. Because families share common diets and environments, their microbiota is expected to be similar. Thus, how shared microbiota influence the transmissibility of NCDs are challenging to investigate, as uncoupling environment from microbiota is difficult.

Obesity is a leading risk factor for many NCDs and there is increasing evidence that obesity has a microbial component. Fecal microbiota transfer (FMT) from genetically predisposed or diet-induced obese animals to germ-free, lean animals causes statistically significant weight gain, indicating that gut microbes are part of the etiology. The risk of post-dieting weight regain in mice is increased by a persistently altered gut microbiota which is transferrable to germ-free mice. Studies suggest that obesity may also be communicable in humans. In a social network study of 12,067 people over 30 years, having an obese friend was associated with a 57% higher chance of being obese, and a 40% higher chance of obesity if a sibling was obese. Moreover, a study of US military families showed that being stationed in a county with high obesity rates was associated with increased body mass index (BMI), whereas those stationed in counties with lower obesity rates had lower BMI. These data are consistent with obesity as a social contagion, representing a shared environment, including diet, lifestyle, as well as microbiota. However, it is difficult to uncouple environment (diet, social habits) from microbiota composition, because they are intimately connected. Currently, microbial transmission of NCDs has only been proven in controlled FMT experiments in animal models.

Obesity is the greatest risk factor for type 2 diabetes (T2D). T2D may also be communicable via the microbiota. Within a year of a T2D diagnosis, spouses have a higher chance of developing T2D, and this trend remains over 3 years following the initial diagnosis. In mice, T2D has a microbially-transferable component, as demonstrated by FMT from mice with T2D into germ-free mice.

Inflammatory bowel diseases (IBDs) are associated with characteristic altered (dysbiotic) microbiota, which can be transferred from diseased humans or mice to healthy animals along with the disease phenotype. Spouses of IBD patients have similar dysbiotic microbiota compositions and a higher rate of disease than accounted for by chance alone, although, like most infectious diseases, the “transmission” rate is not 100%. In India, the rate of ulcerative colitis (UC) is low, yet after moving from India to the UK, USA, and Canada, migrants have higher levels of UC. This change is attributed to “environmental factors” including diet and lifestyle, and the gut microbiota could be a contributing factor. Host genetic predisposition to IBD also plays a role in IBD, with over 200 genetic loci linked to IBD. Many of these, such as NOD2, are linked to immune functions that impact gut microbiota, emphasizing the linkage between host genetics and the microbiota.

PST TiAl Single Crystals & Environment-Friendly Thermoelectric Materials SnTe

by Guang Chen, Member EUAS

Short Biography
Distinguished Professor
Director, MIIT Key Laboratory of Advanced Metallic and Intermetallic Materials Technology
Director, Engineering Research Center of Materials Behavior and Design, Ministry of Education
Nanjing University of Science and Technology
Professional Experience
1999-present: Distinguished Professor, Nanjing University of Science and Technology
2007-2009: Visiting Scientist, Oak Ridge National Laboratory (ORNL), USA
1989-1996: Lecturer/Associate Professor/Professor, Hebei University of Science and Technology
1982-1986: Teaching Assistant, Hebei University of Science and Technology
Fields of Research
Metallic materials and metallurgy engineering; advanced aeronautic and astronautic materials; novel metals and advanced composites; controlled solidification; nanomaterials and amorphous alloys; material structure and phase transformation.
Research Performed
Fundamental and applied studies on mechanical properties of a variety of advanced materials (superalloys, bulk amorphous alloys, TiAl intermetallics, titanium alloys, aluminum alloys and nano-precipitated steels); thermodynamics and phase relationship; kinetics of phase transformation; alloying behavior; alloy design of high-temperature structural materials; material processing and characterization; advanced thermoelectric material system.
Publications
More than 200 academic publications in Nature Materials, Acta Materialia, etc.
Representative honors, awards and recognitions
2018 — Special Allowance of the State Council
2017 — State Innovation Pioneer Award
2016 — State Technological Invention Award

1. PST TiAl Single Crystals

Twinning plays an important role in the deformation of low-symmetry crystals, such as intermetallic compounds, that have inadequate independent slip systems satisfying the von Mises criterion for general deformation. TiAl intermetallics based on the fully lamellar microstructure of γ-TiAl and α_2-Ti_3Al are excellent materials for light-weight high-temperature applications. PST TiAl single crystals with φ = 0° lamellar orientation have

realized a good combination of strength and ductility over a wide temperature range, especially an unprecedented high-temperature performance at 900~950℃. The plastic behavior of PST TiAl single crystals is found to depend strongly on the deformability of the α_2 phase. Twinning in α_2 lamellae plays a key role in accommodating plastic deformation of PST TiAl single crystals to undergo a general homogeneous deformation without cracks. However, the α_2 deformation twins have only been reported in TiAl alloys during compression, and the {2-201}<1-10-4> twinning mechanism in α_2 still remains controversial.

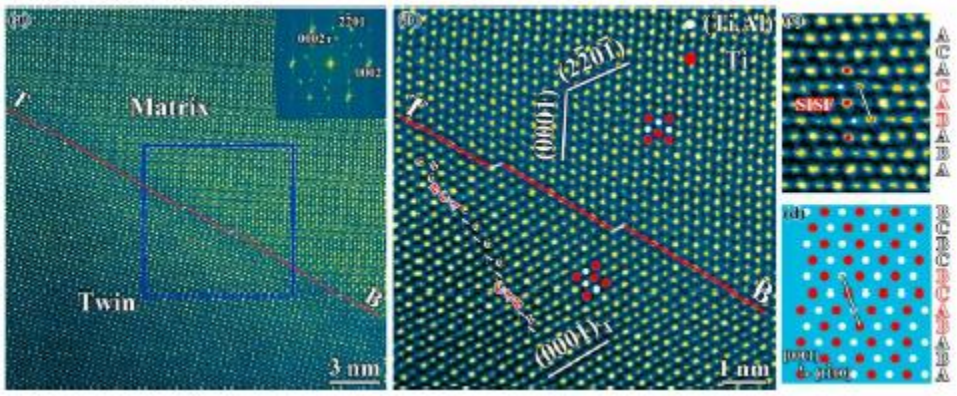

Fig. 1 (a) Atomic resolution HAADF-STEM image of (2-201) twin boundary taken along the [11-20] zone axis. The corresponding fast Fourier transform (FFT) image is inserted. (b) A magnified image enclosed by a blue rectangle in (a), where the coherent twin boundaries and steps are indicated by the red and white lines, respectively. (c) An enlarged image containing I1 type SISF in (b). (d) Schematic illustration of SISF created by the glide of Shockley partial dislocation on the basal plane, as indicated by the white line.

We reveal the formation of the {2-201}<1-10-4> α_2 deformation twins in PST TiAl single crystals after tensile deformation with $\varphi = 0°$ lamellar orientation (i.e., the lamellar boundaries are parallel to the loading axis) at 900 ℃. The fine structure of twin boundary (TB) has been systematically investigated at atomic scale via high-angle annular dark-field (HAADF) imaging using an aberration corrected scanning transmission electron microscope (STEM). The formation mechanism of α_2 deformation twins is clarified by the method of lattice correspondence. These results have been published in the article, *Atomic-scale investigation on the interface structure of {2-201} α_2-Ti_3Al deformation twins in polysynthetically twinned TiAl single crystals*, *Intermetallics*, 128 (2021) 106995.

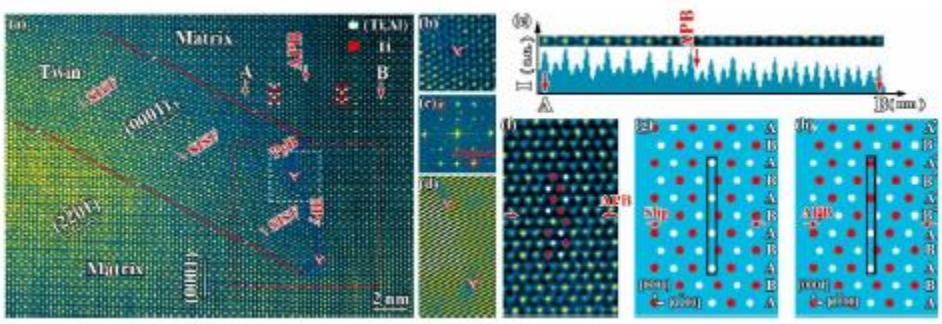

Fig. 2 (a) Atomic resolution HAADF-STEM image of a (2-201) twin tip taken along the [11-20] zone axis. (b) The magnified image of a misfit dislocation enclosed by a white dashed-line rectangle in (a). (c) Corresponding fast Fourier transform (FFT) image enclosed by a red dashed-line rectangle in (a). (d) The corresponding inverse fast Fourier transform (IFFT) pattern, which is obtained by masking the (2-20-1) matrix and (0002) twin diffractions indicated by the red circles in (c). (e) The line intensity profile of atomic columns along the direction of AB in (a), and the corresponding area is inserted. (f) Atomic arrangement near the APB. (g) Atomic projection of α2 along the [11-20] direction. (h) Schematic illustration of APB created by the glide of superpartial dislocation with the vector of 1/6[-2110] on the basal plane indicated by the red arrow in (g).

Our results show that, abundant I1 type basal-plane SISFs are formed and connected with d_{TP} steps in the twins (Fig. 1). Crystallographic analyses reveal that the basal-plane SISFs are not mediated by the glide of Shockley superpartial dislocations (Fig. 2), and complex atomic shuffle and interchange shuffling are responsible for the formation of twinning and basal-plane SISFs in α_2 twins. (Fig. 3). At the vicinity of α_2 twin tip, there are two misfit dislocations recognizable with the extra (220-1) half plane situated in the matrix. The closely adjacent dislocations reflect the high stress concentration at the twin tip. To relieve the stress concentration of the α_2 twin tips, basal-plane APBs are formed at the vicinity of twin tips. The emergence of α_2 deformation twins will open the way for the design of PST TiAl single crystals with higher strength and ductility in the future.

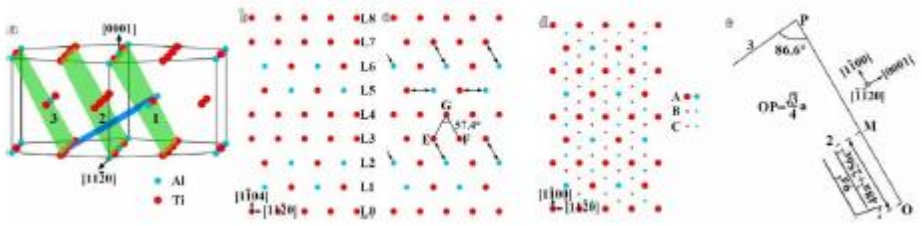

Fig. 3 (a) The schematic diagram of Ti3Al lattice with $D0_{19}$ structure. (b)–(d) Schematic illustration of transformation of the (2-20-1) pyramidal plane of matrix into the (0001) basal plane of twin during the twinning process. (e) The projection of the other two transformed basal planes on the newly created basal plane along the [-1-120] direction.

2. Environment-Friendly Thermoelectric Materials SnTe

Thermoelectric (TE) materials, which are capable to directly convert heat into electricity, may have a significant impact on energy production and utilization. The conversion efficiency of TE base devices, is related to a dimensionless figure of merit, *ZT*, based on the materials' Seebeck coefficient (*S*), electrical conductivity (σ) and thermal conductivity (κ_T) at absolute temperature (*T*). In chalcogenide semiconductors, PbTe is the current state-of-the-art TE materials. However, the high toxicity of Pb limits the wider applications of thermoelectric modules. As a type of isostructural of PbTe, SnTe has been considered as an environmentally friendly candidate. However, energy separation (~0.35 eV) between the light- and heavy-hole bands of SnTe is much larger than that of PbTe (~0.17 eV) at room temperature. Moreover, the lattice thermal conductivity of SnTe is much higher than that of PbTe because of the lighter atomic mass of Sn than that of Pb. Therefore, both electrical and thermal transport properties of SnTe need to be optimized.

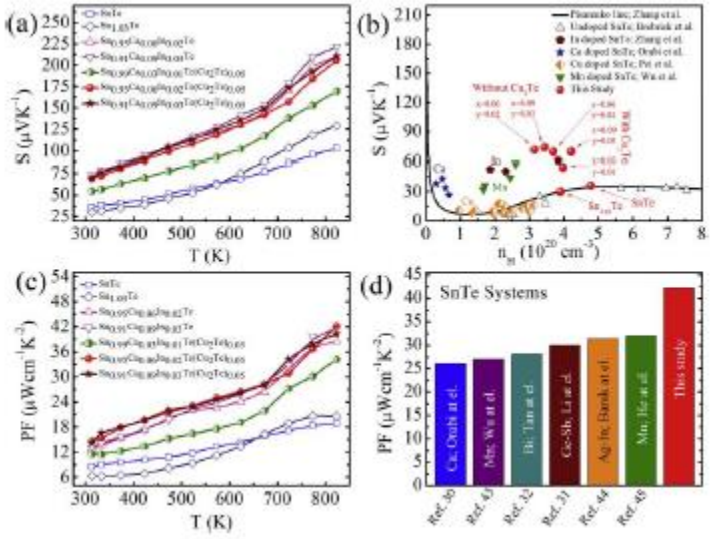

Fig. 4 (a) Temperature dependent Seebeck coefficients; (b) Room temperature Seebeck coefficients as a function of carrier concentration for $Sn_{1.03-x-y}Ca_xIn_yTe$ and $Sn_{1.03-x-y}Ca_xIn_yTe(Cu_2Te)_{0.05}$ samples. For comparison, previously reported data of undoped SnTe, Cu doped, In doped, Ca doped, Mn doped and theoretical Pisarenko curve based on the two-valence-band model are given; (c) power factor as a function of temperature; (d) power factor comparison with different state-of-the-art SnTe systems.

We achieved an ultrahigh power factor and high thermoelectric performance of SnTe via the synergy of resonance levels, band convergence and endotaxial nanostructuring. We found that the coexistence of resonant levels (by In dopant) and band convergence (by Ca dopant) produce remarkable enhancement of Seebeck coefficient and ultrahigh power factor (Fig. 4). The largest power factor reaches as high as ~42.2 $\mu Wcm^{-1}K^{-2}$. Endotaxial Cu_2Te nanostructures were further introduced by a phase separation strategy, which plays a dominant role in reducing the lattice thermal conductivity. Meanwhile, it is revealed that Ca and In codoping enlarges band gap, therefore suppressing bipolar thermal conductivity.

These electronic and thermal effects contribute to a record high *ZT* of ~1.85 at 823 K and a high average *ZT* of 0.67 (Fig. 5). This high performance material is low-cost, earth-abundant and environmentally-friendly, which are essential for the widespread use of thermoelectric modules. Our results have been published in the article, *Realizing high thermoelectric performance in eco-friendly SnTe via synergistic resonance levels, band convergence and endotaxial nanostructuring with Cu_2Te*, *Nano Energy*, 73 (2020) 104832.

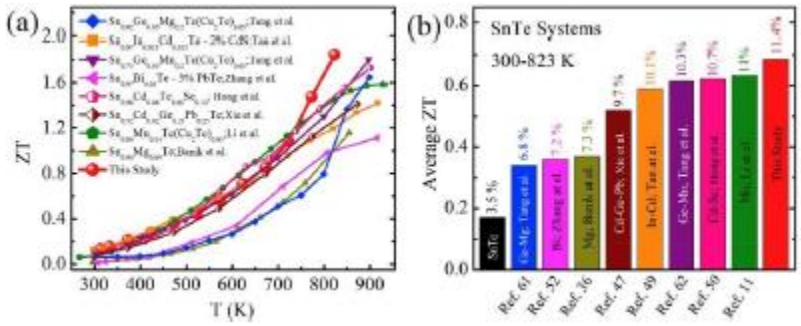

Fig. 5 Thermoelectric properties comparison of $Sn_{0.95}Ca_{0.06}In_{0.02}Te(Cu_2Te)_{0.05}$ in this work with other reported SnTe systems including $Sn_{0.97}In_{0.015}Cd_{0.015}Te$-2%CdS, $Sn_{0.86}Mn_{0.14}Te(Cu_2Te)_{0.05}$, $Sn_{0.94}Mg_{0.09}Te$, $Sn_{0.98}Cd_{0.06}Te_{0.88}Se_{0.12}$, $Sn_{0.52}Cd_{0.02}Ge_{0.25}Pb_{0.25}Te$, $Sn_{0.97}Bi_{0.03}Te$-3%PbTe, $Sn_{0.82}Ge_{0.05}Mg_{0.2}Te(Cu_2Te)_{0.05}$ and $Sn_{0.75}Ge_{0.05}Mn_{0.2}Te(Cu_2Te)_{0.05}$ (a) *ZT* values (b) comparison of ZT_{ave} and thermoelectric conversion efficiency η with a temperature gradient of 300-823 K.

Newton's Law of Cooling: Follow up and Exploration

by Shigenao Maruyama, Member EUAS

Short Biography

Present Affiliation: President, National Institute of Technology, Hachinohe College, Hachinohe 039-1192, Japan

Academic Qualifications

B.Eng. 1977, Department of Mechanical Engineering II, Tohoku University, Japan
M.Sc. 1979, Department of Aeronautics, Imperial College, London University, UK
M.Eng. 1980, Department of Mechanical Engineering, Tohoku University, Japan
PhD 1983, Department of Mechanical Engineering, Tohoku University, Japan

Professional Carriers

1983 Assistant Professor, Institute of High Speed Mechanics, Tohoku University
1988 Visiting Scholar, School of Mechanical Engineering, Purdue University, USA
1989 Associate Professor, Institute of Fluid Science, Tohoku University
1997 Professor, Institute of Fluid Science, Tohoku University.
2005-2006 Specially Appointed Assistant to the President, Tohoku University
2006-2009 Councilor, Tohoku University
2006-2008 Special Advisor to President, Tohoku University
2006-2013 ***Special Advisor for Centenary Events and Alumni, Tohoku University***
2008-2011, 2015-2017 Distinguished Professor of Tohoku University
2016 Visiting Professor, INSA de Lyon
2017- President, National Institute of Technology, Hachinohe College

Awards

Japan Society of Mechanical Engineers (JSME), Award for Young Engineers, 1989
Fluid Science Foundation, Award for Fluid Science, 1995
Heat Transfer Society of Japan (HTSJ), Award for Scientific Contribution, 1998, 2016
JSME Medal for Outstanding Paper, 1999, 2013
HTSJ, Award for Scientific Measurement, 1999
JSME Tohoku Division, Award for Technical Contribution, 2001
Japan Society of Applied Electromagnetic and Mechanics, Best Technical Contribution Award, 2001
JSME Thermal Engineering Division, Award for Academic Achievements, 2001
HTSJ, Award for Technical Contribution, 2002
Societe Francaise de Themique, 2002 International SFT Award, 2002
JSME Thermal Engineering Division, Award for Contribution, 2003
JSME Fellow, 2004
Government of Japan, Japanese Medal of Honor (Medal with Purple Ribbon), 2012
JSME Thermal Engineering Division, Award for Achievements (Research), 2012

Research Activities

Professor Shigenao Maruyama specializes in thermal engineering. He has published more than 10 books and 200 academic research papers, and has acquired 50 patents. He investigated various aspects of fluid flow and energy exchange. Based on the principle that conventional heat transfer and thermal control focuses on the enhancement of heat transfer and temperature control of equipment, he has proposed a novel concept of heat-transfer control, in which the heat transfer is actively enhanced or reduced. The proposed active thermal insulation system and a heat-transfer control device utilizes Peltier effects. His work is interdisciplinary utilizing knowledge from various academic disciplines. He has co-authored and edited Thermodynamics (JSME Text series) [1], one of the bestselling books on thermodynamics for mechanical engineering students in Japan. He has also published a book to educate the public thermal science [2], and a

novel describing accidents in Fukushima Daiichi nuclear plants [3].
Some aspects of his research activities are as follows:
Radiative heat transfer: *Detailed studies on radiative heat transfer, which is energy transfer by infrared or electromagnetic waves, has been carried out. A generalized analysis method to calculate radiative heat transfer was proposed [4], and this method was applied to analyze heat transfer in semi-conductor processes [5] and industrial furnaces. This method was also applied to large-scale environmental energy transfer processes, such as heat transfer in fogs and clouds [6]. Thermal emission from nano-scale structures was also investigated [7]. These results were published in a monograph [8] which is the first textbook on radiative heat transfer in Japan.*
Natural convection: *Natural convection induced by temperature differences in fluid and the gravitational force was studied, and a generalized description was presented [9]. These results were applied to the cooling fins of electronic devices [10]. This research has been extended to understanding large-scale natural convection in oceanography. The up-welling velocity of deep seawater in the ocean which was proposed by Stommel to be a perpetual salt fountain, was successfully measured for the first time in the world [11].*
Active heat-transfer control by Peltier elements: *Peltier elements, used as cooling equipment, have been applied to a heat-transfer control device. This device has been utilized to the heat-transfer control of equipment in a microgravity environment [12], in an active catheter, and in artificial heart muscles [13]. Furthermore, this heat-transfer control has been applied to the fields of oriental medicine and cryosurgery [14]. The concept of heat-transfer control has been expanded to fusion of thermal engineering and medical engineering [15].*

Newton's Law of Cooling: Follow up and Exploration [21]

Isaac Newton's paper, in Latin, on thermal science, *Scala graduum Caloris*, (Scale of the Degree of Heat), published in the Philosophical Transactions (1701) is investigated in detail. This paper contains the descriptions related to Newton's Law of Cooling. We compared the Newton's temperature measurements and physical phenomena to evaluate his measurement lower than the boiling point, or 34 °N in Newton's temperature. In order to follow up the paper, we conducted Newton's experiments on forced convection using a small wind tunnel and tried to reproduce the original results, especially the high-temperature region. We also conducted cooling experiments on natural convection. If the cooling times from the burning temperature of coal (192 °N) to the body temperature (12 °N) were 66, 80.5, and 132 min, the corresponding wind velocities were estimated to be 3.2, 2.2, and 0.7 m/s, respectively. For a wind speed of 0.7 m/s, natural convection cannot be neglected. The study also addresses the reason for why Newton published an anonymous paper on temperature measurement at temperatures higher than the boiling point of the water.

Fig. 1 Isaac Newton (1642-1727) . He was a prominent scientist who lived nearly three centuries ago. His work is momentous and spans many topics, including research on optics, differential and integration, the law of gravitation. In recognition of these scientific achievements, he was interred in Westminster Abbey and an image of him with a reflector telescope that he allegedly invented was included on the back of an old one-pound note. Newton was also interested in thermal science, and the results of his studies were published in the Scientific Journal of the Royal Society in 1701.

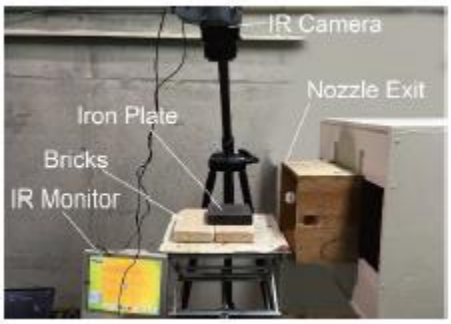

Fig. 2 Small wind tunnel and measurement system for evaluations of Newton's experiment. In order to reproduce Newton's experiment, a small wind tunnel was manufactured, and a cooling experiment was conducted for an iron plate. First, the iron plate was placed in an electrical furnace and heated until it reached a constant temperature. Then, the plate was placed on the bricks in front of the wind tunnel nozzle. The temperatures of the plate were measured every second by a data logger until the plate reached the ambient temperature, and the radiation intensity was measured by an IR camera.

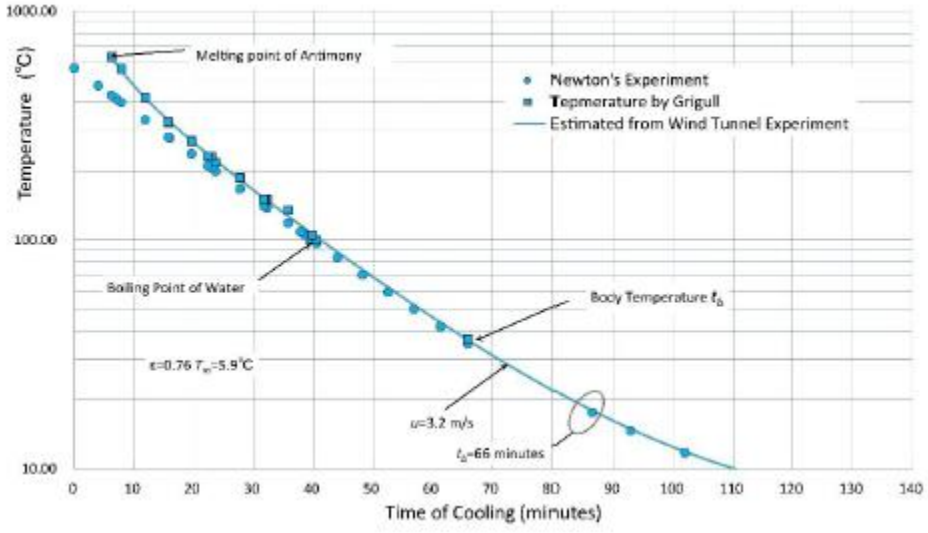

Fig.3 Comparison of Newton's experimental data with our estimation from the empirical formula derived from our wind tunnel experiments. The wind velocities of the estimation were adjusted to fit the experimental data by Newton. We assumed that the cooling time to the body temperature, $t_b = t$ (12 °N), was 66 min, according to Newton's notebook. Newton's temperature estimations are lower than the real temperature because he did not consider the radiative heat transfer. Accordingly, as per Grigull's temperature estimation by metallurgy, the melting point of antimony (Sb), was used for the initial temperature of the estimation of Newton's experiment. We assumed that the ambient temperature T_∞ is 2 °N and the emissivity ε is 0.76, which is the average value of our experiment. The wind velocity was adjusted to fit Newton's experimental data.

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Causes of Irregularities in Trends of Global Mean Surface Temperature since the Late 19th Century

by Chris Folland, Member EUAS

Short Biography

Chris K. Folland, Retired UK Met Office Science Fellow, and Universities of East Anglia, UK, Gothenburg , Sweden, and Southern Queensland, Australia

The author has had a varied career in meteorology since 1968, mostly at the UK Met Office, after becoming a Fellow of the Royal Meteorological Society in 1967. He joined the Operational Instrumentation Branch in 1969 and took charge of a small group researching the development of surface meteorological instruments, particularly those measuring temperature and humidity on land and at sea. This included probably the first successful automated measurements of atmospheric humidity on a buoy. The author became involved with the World Meteorological Organisation (WMO), providing scientific input to the WMO Working Group on Reference Psychrometry. An instrumental background was to prove valuable for later research on correcting time-varying observed sea surface temperature (SST) biases, important for accurate climate change estimates.

The author joined the Met Office branch involved in climate change and UK monthly forecasting, Here, he co-authored a Nature paper in 1974 on the emerging Sahel drought. From 1976-1980, the author led a group working on hydrometeorological research and commercial consultancy. A key activity was working with hydrologists, hydraulics experts and prominent civil engineers to provide meteorological, mainly extreme rainfall statistics, input to a pioneering computerised model and manual for the hydraulic design of storm sewers, an activity sponsored by the UK National Water Council and its Department of the Environment (DOE). Another activity involved research for the WMO Working Group on Precipitation Evaporation and Soil Moisture to develop a physical model to quantitatively explain the long-standing problem of the systematic losses of rainfall from conventional raingauges and to test these ideas in the field. This included working with hydrologists at the UK Institute of Hydrology and led to a new raingauge design to minimise systematic rainfall and snowfall losses from conventional raingauges. This design was initially marketed as the Folland Sevruk Strangeways (FSS)100 tipping bucket raingauge in the late 1980s and is made today as the ARG100 raingauge marketed by several companies. This activity was helped by membership of the Royal Society sub-group on Hydrology (1979-82). For both research activities the author was awarded the Royal Meteorological Society's Hugh Robert Mill Medal and Prize in 1985. The author was also involved with hydrologists in the Institute of Civil Engineers on follow up research to the landmark 1975 UK Flood Studies Report and carried out hydrometeorological consultancy jobs for clients as part of the commercial consultancy work of his group. His most recent scientific work in hydrometeorology published in 2015, (in the Met Office Hadley Centre, see below) was a paper identifying the climatic causes of winter half year (October-March) meteorological and hydrological droughts in southern UK.

Causes of Irregularities in Trends of Global Mean Surface Temperature since the Late 19th Century

Chris K. Folland, Olivier Boucher, Andrew Colman, David E. Parker

Science Advances, 4

Abstract

The time series of monthly global mean surface temperature (GST) since 1891 is successfully reconstructed from known natural and anthropogenic forcing factors, including internal climate variability, using a multiple regres- sion technique. Comparisons are made with the performance of 40 CMIP5 models in predicting GST. The relative contributions of the various forcing factors to GST changes vary in time, but most of the warming since 1891 is found to be attributable to the net influence of increasing greenhouse gases and anthropogenic aerosols. Separate statistically independent analyses are also carried out for three periods of GST slowdown (1896–1910, 1941–1975, and 1998–2013 and subperiods); two periods of strong warming (1911–1940 and 1976–1997) are also analyzed. A reduction in total incident solar radiation forcing played a significant cooling role over 2001–2010. The only serious disagreements between the reconstructions and observations occur during the Second World War, especially in the period 1944–1945, when observed near-worldwide sea surface temperatures (SSTs) may be significantly warm-biased. In contrast, reconstructions of near-worldwide SSTs were rather warmer than those observed between about 1907 and 1910. However, the generally high reconstruction accuracy shows that known external and internal forcing factors explain all the main variations in GST between 1891 and 2015, allowing for our current understanding of their uncertainties. Accordingly, no important additional factors are needed to ex- plain the two main warming and three main slowdown periods during this epoch.

Experiment design of the International CLIVAR C20C+ Detection and Attribution project

Dáithí A. Stonea, Nikolaos Christidisd, Chris Follandd, Sarah Perkins-Kirkpatricke, Judith Perlwitzg, Hideo Shiogamah, Michael F. Wehnera, Piotr Wolskii, Shreyas Choliaa, Harinarayan Krishnana, Donald Murrayg, Oliver Angélila,e, Urs Beyerlej, Andrew Ciavarellad, Andrea Dittusf, Xiao-Wei Quang, Mark Tadrossi

Weather and Climate Extremes, 24

Abstract

There is a growing research interest in understanding extreme weather in the context of anthropogenic climate change, posing a requirement for new tailored climate data products. Here we introduce the Climate of the 20th Century Plus Detection and Attribution project (C20C + D&A), an international collaboration generating a product specifically intended for diagnosing causes of changes in extreme weather and for understanding un- certainties in that diagnosis. The project runs multiple dynamical models of the atmosphere-land system under observed historical conditions as well as under naturalised versions of those observed conditions, with the latter representing how the climate system might have evolved in the absence of anthropogenic interference. Each model generates large ensembles of simulations with different initial conditions for each historical scenario, providing a large sample size for understanding interannual variability, long-term trends, and the anthropogenic role in

rare types of weather. This paper describes the C20C + D&A project design, implementation, strengths, and limitations, and also discusses various activities such as this special issue of *Weather and Climate Extremes* dedicated to "First results of the C20C + Detection and Attribution project".

CMIP5 Climate Models Overestimate Cooling by Volcanic Aerosols

Petr Chylek, Chris Folland, James D. Klett and Manvendra K. Dubey

Geophysical Research Letters,47

Abstract

We compare projections of the observed hemispherical mean surface temperature (HadCRUT4.6.0.0) and the ensemble mean of CMIP5 climate models' simulations on a set of standard regression model forcing variables. We find that the volcanic aerosol regression coefficients of the CMIP5 simulations are consistently significantly larger (by 40–49%) than the volcanic aerosol coefficients of the observed temperature. The probability that the observed differences are caused just by chance is much less than 0.01. The overestimate is due to the climate models' response to volcanic aerosol radiative forcing. The largest overestimate occurs in the winter season of each hemisphere. We hypothesize that the models' parameterization of aerosol-cloud interactions within ice and mixed phase clouds is a likely source of this discrepancy. Furthermore, the models significantly underestimate the effect of solar variability on temperature for both hemispheres.

Changes in the future summer Mediterranean climate: contribution of teleconnections and local factors

Monika J. Barcikowska, Sarah B. Kapnick, Lakshmi Krishnamurty, Simone Russo, Annalisa Cherchi and Chris K. Folland

Earth System Dynamics, 11, 161–181

Abstract

This study analyzes future climate for the Mediterranean region projected with the high-resolution coupled CM2.5 model, which incorporates a new and improved land model (LM3). The simulated climate changes suggest pronounced warming and drying over most of the region. However, the changes are distinctly smaller than those of the CMIP5 multi-model ensemble. In addition, the changes over much of southeast and cen- tral Europe indicate very modest warming compared to the CMIP5 projections and also a tendency toward wetter conditions. These differences indicate a possible role of factors such as land surface–atmospheric interactions in these regions. Our analysis also highlights the importance of correctly projecting the magnitude of changes in the summer North Atlantic

Oscillation, which has the capacity to partly offset anthropogenic warming and drying over the western and central Mediterranean. Nevertheless, the projections suggest a decreasing influence of local atmospheric dynamics and teleconnections in maintaining the regional temperature and precipitation balance, in particular over arid regions like the eastern and southern Mediterranean, which show a local maximum of warming and drying. The intensification of the heat low in these regions rather suggests an increasing influence of warming land surface on the local surface atmospheric circulation and progressing desertification.

Pen Portraits of Presidents – Sir Basil John Mason

Chris K. Folland and John F. B. Mitchell

Weather, 75, 26-29

Introduction

Sir Basil John Mason known as John Mason, Director General of the Meteorological Office for the long and transformative period 1965–1983, was the one of the most influential and charismatic meteorologists in history. He had a profound influence in developing the new opportuni- ties that largely created the recent and current generation of meteorologists in the UK, and his global influence was just as important. He also established cloud physics as an important discipline in its own right.

The authors of this pen portrait attribute our careers to the visionary expansion in meteorological and climatological research in the Met Office that Sir John initiated after taking up leadership of the Met Office in 1965. In the remainder of this paper, we owe much to the biographical memoir by Browning (2016) and Sir John's autobio- graphical reminiscences (Mason, 2010), as well as to a number of colleagues and our own memories. We also used the brief biog- raphy in *Weather* published by Jonas (2015). John Mason was born in Norfolk in the village of Docking, east of Hunstanton, on 18 August 1923. He attended the nearby Fakenham Grammar School, and World War II began when he was in the sixth form of secondary school. As those who might have taught him had gone off to war, he had no formal teaching in mathematics or physics for his Higher School Certificate (the equivalent of today's A-levels), and he became largely self-taught. There was, however, a very good biology teacher at his school, and in 1941 John Mason won a scholarship to University College, Nottingham, on the strength of his biology exam results. Once at university, he took up physics and mathematics, a testa- ment to the quality of his self-directed learning. He was called up in 1944 before he could finish his degree, when he joined the Royal Air Force as a radar officer and became an instructor. At the early age of 21 he became Officer-in-charge of Signals and Telecommunications in Batavia (now Jakarta, Indonesia) in the then Dutch East Indies. After the war he completed his physics degree at Nottingham University, gaining first-class honours in 1947. He was subsequently awarded a Shirley Research Fellowship, work- ing on surface physics at Nottingham for a year, in anticipation of going on to complete a PhD. However, an attractive job opportu- nity arose, and he left after one year with an MSc, having published two research papers
on surface tension.

Computational Hardware & Theoretical Methods for Molecular Quantum Mechanics

by Henry F. Schaefer, Member EUAS

Short Biography

Henry F. Schaefer III was born in Grand Rapids, Michigan. He attended public schools in Syracuse (New York), Menlo Park (California), and Grand Rapids (Michigan), graduating from East Grand Rapids High School. In 2018 Professor Schaefer received the Alumnus/Alumna of the Year Award from East Grand Rapids High School. He received his B.S. degree in chemical physics from the Massachusetts Institute of Technology and Ph.D. degree in chemical physics from Stanford University. For 18 years he served as a professor of chemistry at the University of California, Berkeley. During the 1979-1980 academic year he was also Wilfred T. Doherty Professor of Chemistry and inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. Dr. Schaefer is currently Graham Perdue Professor of Chemistry and Director of the Center for Computational Quantum Chemistry at the University of Georgia. He is simultaneously Professor of Chemistry, Emeritus, at the University of California at Berkeley. His other academic appointments include Professeur d'Echange at the University of Paris (1977), Gastprofessur at the Eidgenössische Technische Hochshule (ETH), Zürich (1994, 1995, 1997, 2000, 2002, 2004, 2006, 2008, 2010), David P. Craig Visiting Professor at the Australian National University (1999), and Visiting Professor at the Ludwig Maximilians University (LMU) Munich (2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019).

Schaefer is the author of more than 1600 scientific publications, with a large majority appearing in the *Journal of Chemical Physics*, *Journal of the American Chemical Society* or the *Journal of Physical Chemistry*. A total of 300 scientists from 35 countries gathered in Gyeongju, Korea for a six-day conference in February, 2004 with the title "Theory and Applications of Computational Chemistry: A Celebration of 1000 Papers of Professor Henry F. Schaefer III." In May 2010, the University of California at Berkeley hosted a large international conference in Professor Schaefer's honor, the title of the conference being "Molecular Quantum Mechanics: From Methylene to DNA and Beyond." Simultaneous with the Berkeley conference was published the book *Selected Papers of Henry F. Schaefer III*, Edited by R. J. Bartlett, T. D. Crawford, M. Head-Gordon, and C. D. Sherrill. In May 2014 the Peking University Graduate School sponsored a large conference in honor of Professor Schaefer and Professor Leo Radom in Shenzhen, China. In August 2019, the American Chemical Society Division of Physical Chemistry held a five-day symposium titled "Computational Quantum Chemistry: from Promise to Prominence," in honor of Dr. Schaefer in San Diego, California. A symposium in Professor Schaefer's honor is planned for December 2021 at the International Chemical Congress of Pacific Basin Societies (PACIFICHEM) in Honolulu, Hawaii.

Critical to Professor Schaefer's scientific success has been a brilliant array of students and coworkers; including 79 undergraduate researchers who have published papers with him, 127 successful Ph.D. students (plus 14 in progress), 55 postdoctoral researchers, and 81 visiting professors who have spent substantial time in the Schaefer group. A number of his students have gone on to positions of distinction in industry (Accelrys, Adesis, ALTANA, American Cyanamid, AstraZeneca, AT&T, Avaya, Bicerano and Associates,

Castle Hill Gaming, Chemical Abstracts, Clariant, Computational Geosciences, Coraid, DeNovaMed, Deutsche Bank, Dow Chemical, ELANTAS, Electronic Arts, Endress-Hauser, EnerDel, First Source Research, GAUSSIAN, Goodrich, Google, Henkel, Hewlett-Packard, Hughes Aircraft, IBM, ICON, Komag, Locus Pharmaceuticals, Lonza Pharma & Biotech, Materials Design, McKesson Corp, Mobil Research, Molecular Simulations, Monsanto, Nimble Storage, OpenEye, OSI Software, PartnerRe, Pfizer, Pharmaceutical Research Associates, Polaroid, Proctor & Gamble, Q-CHEM, Reagens Deutschland, Ricoh, RWDC Bioplastics, Schroedinger, SciCo, Sugen, Treventis, Universal Display Corporation, VALIS, WaveSplitter Technologies, Xcellence LLC, and Xenon Pharmaceuticals). Four of his graduated Ph.Ds have started their own companies.

Several of Schaefer's former students have gone on to successful careers in government laboratories, including the Australian National University Supercomputer Center, Environmental Protection Agency (EPA), Joint Institute for Laboratory Astrophysics (JILA), Lawrence Berkeley National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Molecular Sciences Software Institute, NASA Ames, National Cancer Institute, National Center for Disease Control, National Institute of Environmental Health Sciences, National Institutes of Health (Bethesda), National Research Council of Canada (Ottawa), Naval Research Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Pittsburgh Supercomputing Center, Sandia National Laboratories, and the Savannah River National Laboratory. Charles Blahous went directly from his Ph.D. studies with Dr. Schaefer to the position of American Physical Society Congressional Scientist Fellow, and eventually to positions of significant importance in the U.S. political system (chief of staff for Senator Alan Simpson of Wyoming and later for Senator Judd Gregg of New Hampshire; and Executive Director of President George W. Bush's Bipartisan Committee to Strengthen Social Security; see *Wall Street Journal* article April 22, 2005). Dr. Blahous is currently Research Fellow at the Hoover Institution, Stanford University, and J. Fish and Lillian P. Smith Chair at the Mercatus Center, George Mason University. He was appointed by President Barack Obama to the Board of Trustees for Social Security and Medicare.

Many of Dr. Schaefer's students have accepted professorships in universities, including the University of Alabama at Birmingham, University of Arizona, Beijing Normal University, Budapest University (Hungary), University of California at Merced, City University of New York, University of Concepcion (Chile), Duke University, Emory University, Fatih University (Istanbul, Turkey), Georgia Tech, University of Georgia, University of Giessen (Germany), University of Girona (Spain), University of Grenoble (France), University of Guelph (Ontario), Hacettepe University (Ankara), University of Heidelberg (Germany), University of Illinois-Chicago, University of Illinois-Urbana, Indian Association for the Cultivation of Science (Calcutta), Indiana University-Purdue University at Indianapolis, Johns Hopkins University, Keio University (Japan), University of Kentucky, Lehigh University, University of Manchester (England), University of Marburg (Germany), University of Massachusetts, University of Memphis, University of Michigan, University of Mississippi, National Tsing Hua University (Taiwan), University of North Dakota, Ohio State University, Osaka University (Japan), University of Ottawa (Canada), University of Paris - Sud (France), Pennsylvania State University, University of Pittsburgh, Pohang Institute of Science and Technology (Korea), Portland State University, Rice University, Rikkyo University (Tokyo), Scripps Research Institute, University of South Florida, St. Andrew's University (Scotland), St. Petersburg State

University (Russia), Stanford University, University of Stirling (Scotland), University of Stockholm (Sweden), University of Tasmania (Australia), Technical University of Munich (Germany), Texas A&M University, the University of Texas at Arlington, University of Trondheim (Norway), University of Tübingen (Germany), Ulsan National University of Science and Technology (Korea), and Virginia Tech.

Dr. Schaefer has been invited to present plenary lectures at more than 300 national or international scientific conferences. He has delivered endowed or named lectures or lecture series at more than 60 major universities, including the Kenneth S. Pitzer Memorial Lecture at Berkeley, the Israel Pollak Distinguished Lectures at the Technion - Israel Institute of Technology, Haifa, the C. V. Raman Memorial Lecture in Calcutta, India, the Per-Olov Lowdin Lectures at the University of Uppsala, Sweden, and the Jan Almlöf/Odd Gropen Lectures in Norway. He is the recipient of 31 honorary degrees. He served as Editor-in-Chief of the London-based journal *Molecular Physics* for ten years (1995-2005). He is currently Associate Editor for the journal *Physical Chemistry Chemical Physics.* He was also the longest serving President of the World Association of Theoretical and Computational Chemists, from 1996 to 2005. His service to the chemical community includes the chairmanship of the American Chemical Society's Subdivision of Theoretical Chemistry (1982) and Division of Physical Chemistry (1992). At the 228th National Meeting of the American Chemical Society (Philadelphia, August, 2004) the Division of Computers in Chemistry and the Division of Physical Chemistry co-sponsored a four-day "Symposium in Honor of Henry F. Schaefer's 60th Birthday." The book *Theory and Applications of Computational Chemistry: The First Forty Years* (1308 pages, Elsevier) was published in 2005 in honor of Professor Schaefer.

Professor Schaefer's major awards include the American Chemical Society Award in Pure Chemistry (1979, "for the development of computational quantum chemistry into a reliable quantitative field of chemistry and for prolific exemplary calculations of broad chemical interest"); the American Chemical Society Leo Hendrik Baekeland Award (1983, "for his contributions to computational quantum chemistry and for outstanding applications of this technique to a wide range of chemical problems"); the Schrödinger Medal (1990); the Centenary Medal of the Royal Society of Chemistry (London, 1992, as "the first theoretical chemist successfully to challenge the accepted conclusions of a distinguished experimental group for a polyatomic molecule, namely methylene"); the American Chemical Society Award in Theoretical Chemistry (2003, "for his development of novel and powerful computational methods of electronic structure theory, and their innovative use to solve a host of important chemical problems"). In 2003 he also received the annual American Chemical Society Ira Remsen Award, named after the first chemistry research professor in North America. The Remsen Award citation reads "For work that resulted in more than one hundred distinct, critical theoretical predictions that were subsequently confirmed by experiment and for work that provided a watershed in the field of quantum chemistry, not by reproducing experiment, but using state-of-the-art theory to make new chemical discoveries and, when necessary, to challenge experiment."

The Journal of Physical Chemistry published a special issue in honor of Dr. Schaefer on April 15, 2004. In 2009 and 2010, the journal *Molecular Physics* published seven separate issues in honor of Professor Schaefer. He was elected a Fellow of the American Academy of Arts and Sciences in 2004. He was the recipient of the prestigious Joseph O. Hirschfelder Prize of the University of Wisconsin for the academic year 2005-2006. He

became a Fellow of the Royal Society of Chemistry (London) in 2005. He was among the inaugural class of Fellows of the American Chemical Society, chosen in 2009. He earlier became a Fellow of the Alfred P. Sloan Foundation, John S. Guggenheim Foundation, American Physical Society, and American Association for the Advancement of Science. In April 2011 he received the Ide P. Trotter Prize of Texas A&M University. Recent recipients of this prestigious award have included Nobelists Charles Townes, William Phillips, Francis Crick, Steven Weinberg, and Roald Hoffmann. In 2012 he received the Alexander von Humboldt Award. In March 2012 Professor Schaefer received the $20K SURA Distinguished Scientist Award, given to the outstanding scientist in any field in the southern USA, from Missouri to Texas to Florida to Virginia. In April 2013, at the Chemical Heritage Foundation in Philadelphia, Dr. Schaefer received the Chemical Pioneer Award of the American Institute of Chemists. In January 2014 he was named by *The Best Schools* as one of "The 50 Most Influential Scientists in the World Today." In March 2014 he received the American Chemical Society Peter Debye Award in Physical Chemistry. In February 2016 he was elected an Honorary Fellow of the Chemical Research Society of India. In May 2019, he received the Gold Medal of the American Institute of Chemists. Seven of the previous 14 recipients of the AIC Gold Medal received the Nobel Prize. Also in May 2019 Dr. Schaefer received the ACS Charles H. Stone Award.

For 40 years Professor Schaefer has been one of the most highly cited scientists in the world. The Science Citation Index reports that his research had been cited more than 75,000 times. Professor Schaefer's Thomson-Reuters H-index is currently 121. He has published 165 Citation Classic Papers. His research involves the use of state-of-the-art computational hardware and theoretical methods to solve important problems in molecular quantum mechanics.

Professor Schaefer is also well known as a student of the relationship between science and religion. One or more of the 500+ lectures in his popular lecture series on this important topic have been presented at most major universities in North America, including Harvard, Stanford, Berkeley, M.I.T., Yale, Princeton, and the Universities of Alberta and Toronto. The Veritas Forum has called on Professor Schaefer to give major lectures at 18 of its conferences. Dr. Schaefer has also presented science/religion lectures in many universities abroad, including those in Ankara, Bandung (Indonesia), Bangalore, Beijing, Belo Horizante, Berlin, Bern, Bratislava, Brisbane, Budapest, Cajamarca (Peru), Cambridge (England), Canberra, Cape Town, Chengdu, Chennai (Madras), Christchurch, Cluj-Napoca, Kochi (Cochin), Delhi, Durban, Florence, Goa, Guangzhou, Guilin, Guwahati, Heidelberg, Hong Kong, Hyderabad, Istanbul, Izmir, Kanpur, Karlsruhe, Kolkata (Calcutta), Krakow, Kunming, Lanzhou, Lausanne, Leipzig, London, Lucknow, Montevideo (Uruguay), Mumbai (Bombay), Munich, Oxford (England), Paris, Plovdiv, Prague, Pondicherry, Pune, Rome, Santiago (Chile), Sarajevo, Seoul, Shanghai, Shenzhen, Shillong, Simferopol, Singapore, Sofia, Split, St. Petersburg, Strasbourg, Sydney, Szeged, Taipei, Tianjin, Tokyo, Trivandrum, Turin, Uppsala, Urumqi, Varanasi (Banares), Vienna, Warsaw, Wuhan, Wuxi, Xiamen, Zagreb, and Zurich. His continuously evolving lecture "The Big Bang, Stephen Hawking, and God" appears in many locations and in several languages on the worldwide web. This lecture has been one of the most popular articles about science on the web in recent years, as discussed in Michael White and John Gribbin's best selling biography of Professor Hawking (pages 314-315 of the 2002 edition). A brief spiritual biography (through 1991, written by Dr. David Fisher) of

Professor Schaefer may be found on pages 323 – 326 of the book *More Than Conquerors*, edited by John Woodbridge (Moody Press, Chicago 1992).

Professor Schaefer was featured (page 62) in the December 23, 1991 cover story of *U.S. News & World Report*, entitled "The Creation: Religion's Search for a Common Ground with Science." Therein he stated: "The significance and joy in my science comes in those occasional moments of discovering something new and saying to myself 'So that's how God did it.' My goal is to understand a little corner of God's plan."

Professor Schaefer is a Fellow of the American Scientific Affiliation, and an extended Profile of him appears in the *ASA Newsletter*, Volume 43, Number 6, 2001. On April 24, 2002 Dr. Schaefer received the Erick Bogseth Nilson Award, given to an outstanding university professor in North America, by the organization Christian Leadership. In May 2005 Dr. Schaefer was elected a Corresponding Member of the Catholic Academy of Sciences in the USA. In November 2014, he was elected a member of the Executive Council of the American Scientific Affiliation, the largest organization of Christians in the sciences in North America. An article featuring Professor Schaefer entitled "A Chemist and God", appeared in the October 18, 2008 issue of *World* magazine. An eight page interview of Schaefer appears in the 2010 book *Open Questions*: *Diverse Thinkers Discuss God, Religion, and Faith*. On January 13, 2013 *The Best Schools* included Schaefer in its list of the "Fifty Smartest People of Faith." He is featured on pages 585-587 of *Encyclopedia of Christianity and Science* (Zondervan, 2017). At the University of Georgia Professor Schaefer teaches an oversubscribed freshman seminar *Science and Christianity: Conflict or Coherence?* Dr. Schaefer's book with the same title will have its Third Edition published in 2021. The book reached position #84 on the best-selling list of Amazon.com.

Old Remagnetizations of Carbonate Rocks

by Rob Van der Voo, Member EUAS

Short Biography

Education: B. Sc. (1961, Geology), M.Sc. (1965, Geology), M.Sc. (1969, Geophysics), Ph.D. (1969, Geology and Geophysics), all at the University of Utrecht, the Netherlands. Dissertation title: "Paleomagnetic evidence for the rotation of the Iberian Peninsula"

Professional positions

University of Michigan:	*2016- present*	*Thurnau Emeritus Professor*
	2016-present	*Frank H T Rhodes Emeritus Professor*
	2003- 2016	*Frank H T Rhodes Professor*
	1994-2016	*Thurnau Professor*
	1998-2003	*Director Honors Program*
	1991-1995	*Chairman of Geological Sciences*
	1981-1988	*Chairman of Geological Sciences*
	1979-2016	*Professor*
	1975-1979	*Associate Professor*
	1972-1975	*Assistant Professor*
	1970-1972	*Visiting Assistant Professor*
Universities of Utrecht & Delft, the Netherlands	*1997-1998*	*Visiting Professor*
Instituto Jaume Almera Barcelona, Spain	*1990-1991*	*Visiting Research Scientist*
Norwegian Acad. Sci. Lett.	*2010-2011*	*Centre Advanced Study – Fellow*
Chinese Academy Sciences	*Spring 2012*	*Einstein Visiting Professor*
Greenland Geological Survey, Copenhagen	*Summer 1985*	*Research Scientist*
U-Texas at Arlington	*Oct. 1984*	*Guest Professor*
University of Kuwait	*Dec. 1979*	*Guest Professor*
University of Rennes	*Jan-Aug 1977*	*Fellow of the C.N.R.S.*
ETH-Zürich	*Apr-Aug 1978*	*Visiting Professor*
Lamont-Doherty Geol. Obs.		
Columbia University	*May-Dec 1976*	*Senior Research Fellow*
University of Utrecht	*1964-1970*	*Research Assistant & Associate*

Honors and Awards *Utrecht University, 1969, Ph.D. degree awarded Cum Laude; University of Michigan, 1976, Henry Russel Award; Elected to Royal Academy of Sciences, the Netherlands, as correspondent, 1979; Elected Fellow of the American Geophysical Union, 1982; University of Michigan, 1990, Distinguished Faculty Achievement Award; University of Michigan, Excellence in Education Awards 1991, 1992, 1993.Geological Society of America, 1992, G.P. Woollard Award; Elected to Royal Norwegian Society of Sciences and Letters, 1995; A.V. Cox Lecturer, American Geophysical Union Spring Meeting, 1997; University of Michigan, LS&A Distinguished Faculty Lecturer, 1998; LSA named Collegiate Professor (Frank H. T. Rhodes), 2003-present.Benjamin Franklin Medal in Earth Science, Franklin Institute, 2001; University of Michigan, M. and H. Sokol Faculty Award in the Sciences, 2006; European Geosciences Union, Petrus Peregrinus Medal, 2014.*

Principal Research Interests

Pre-Mesozoic paleomagnetism and plate tectonics; tectonics of the Caribbean and Mediterranean areas, Hercynian Europe and central Asia; rock magnetism and electron microscopy of sediments and ocean-floor basalts; Neogene magnetostratigraphy and environmental conditions of northeast Tibet; Structure and tectonics of orogenic belts; Oroclinal bending; General geodynamics as related to mantle tomography and paleogeography.

Professional Service (incl. Scientific Societies)

Geological Society of America: Past-president (2005-2006), President (2004), Vice President (2003) and

Councillor (1999-2001, 2003-06), Budget and Finance Committees, Executive Committee Member (2000, 2003-06), Assoc. Editor Geol. Soc. America Bulletin (1981-83; 1989-93), Geology (1975-81; 1990-92), member Arthur Day Medal Committee (1984-86), G.P. Woollard Medal Committee (1994-96), Annual Program Committee Member (1999) and Chair (2000-02), Nominating Committee Chair (2001), Congressional Fellow Selection Committee (2003), Geology and Public Policy Committee (2003); Public Service Award Committee (2005).
American Geophysical Union: President and President Elect Geomagnetism and Paleomagnetism Section and AGU Council Member (1988-92), Editor Geophys. Res. Lett. (1983-87), Assoc. Editor Reviews of Geophysics (1988-91) and Tectonics (1985-96), past member of Committee on Education and Human Resources, Macelwane Award Committee, Fellowship Committee, Bucher Medal Committee, Fleming Medal Committee, Publications Committee, Various Editor Search Committees, Convenor of special symposia (1978-93, 2005, 2008) at Annual meetings
Other (active/recent): Assoc. Editor Tectonophysics, Chairman Advisory Board of the Center for Earth Evolution and Dynamics (CEED), University of Oslo.
Other (past): Editor-in-Chief Earth Science Reviews (2006 - 2009), Editor Earth and Planetary Science Letters (1992-2003); Editorial Board Terra Nova; Editorial Board Journal of Geodynamics. Convenor IAGA and IUGG meeting symposia (1977, 1979, 1981, 1989, 1999, 2001); Convenor of symposia in 1989 International Geological Congress and the European Geosciences Union meetings (1990, 1996, 2000, 2003, 2011). Convenor symposium GDP-04 Palaeozoic-Mesozoic earth geography: Palaeomagnetic, faunal and facies constraints, at International Geological Congress, Oslo, 2008. Member Council of Scientific Society Presidents (2003-2004), Advisory Board member (2002 – 2014) of the Canadian Institute for Advanced Research (CIFAR) – Earth System Evolution Program (ESEP), Advisory Board Member Center for Crust to Core Fluid Systems (CCFS) Macquarie University, Sydney, Australia, May 2013. Member advisory committee of the Institute for Rock Magnetism, University of Minnesota; Panel member of National Research Council Associateship program; NSF Earth Science Division panel (1982-85); NSF panel to evaluate Distinguished Teaching Scholar nominations, December 2004; Member U. S. Geodynamics Committee (National Research Council); International Lithosphere Commission member, and Chairman of Working Group 2 on "Phanerozoic Plate Motions and Orogenesis" (1981-1985); National Academy of Sciences Subcommittee on IAGA (1984). Past chair of visitation committee of the Vening Meinesz Research School of Geodynamics, Delft and Utrecht, the Netherlands. Past member of evaluation/visitation committees for departments of geology at University of Pittsburgh; University of Minnesota; Bowling Green State University; Ohio State University; Indiana University; Harvard University; Science Foundation of Sweden; (combined) VSNU teaching visitation of Dutch/Belgian (Flemish) University Departments of Earth Science.
EU Academy of Sciences (EUAS): Member.

Old Remagnetizations of Carbonate Rocks

Rob Van der Voo, University of Michigan, abstract for Nordic paleomagnetism meeting, with collaboration of Prof. Ben van der Pluijm

Many unmetamorphosed carbonates all over the world are demonstrably remagnetized, with the age of the secondary magnetizations typically close to that of the nearest orogeny in space and time. This observation did not become compelling until the mid-1980's, when the incremental fold test revealed the Appalachian carbonates to carry a syn-deformational remanence of likely Permian age (Scotese et al., 1982, *Phys. Earth Planet. Int.*, v. 30, p. 385-395; see also Cederquist et al., 2006, *Tectonophysics* v. 422, p. 41-54).

Since that time scores of Appalachian rocks have added results to the growing database of paleopoles representing remagnetizations, which form a cloud of results surrounding the Late Carboniferous to Early Triassic reference poles of the Laurentian APWP. Remagnetizations in other locales and with inferred ages coeval with regional orogenies (e.g., Taconic, Sevier/Laramide, Variscan, Indosinian) are also ubiquitous. To be able to transform this cornucopia into valuable anchor-points

on the APWP would be highly desirable. This may indeed become feasible, as will be explained next.

Recent studies of faulted and folded carbonate-shale sequences have shown that this deformation enhances the illitization of smectite (Haines & van der Pluijm, 2008, *Jour. Struct. Geol.*, v. 30, p. 525-538; Fitz-Diaz et al., 2014, *International Geol. Review*, v. 56, p. 734-755). ^{39}Ar-^{40}Ar dating of the authigenic illite – neutralizing any detrital illite contribution by taking the intercept of a mixing line – yields, therefore, the age of the deformation. We know that this date is also the age of the syn-(!)deforma-tional remanence and voilà, we have the age of the corresponding paleopole. Results so far are obtained for the Canadian and U.S. Rocky Mountains and for the Spanish Cantabrian carbonates (Tohver et al., 2008, *Earth Planet. Sci. Lett*., v. 274, p. 524-530) and make good sense in accord with geological knowledge.

Knowing remagnetization ages in millions of years ago not only increases support for APWP constructs, but also for the analysis of along-strike and cross-strike trends, for instance. Such trends, in turn, will have the potential to unravel tectonic collision scenarios.

Tectonic History of the Earth

Rob van der Voo and Trond H. Torsvik

Section 2.2 from the Publication, *Geomagnetism, Aeronomy and Space Weather: A Journey from the Earth's Core to the Sun,* edited by Mioara Mandea, Monika Korte, Andrew Yau, Eduard Petrovsky. Cambridge University Press.

As time goes by, fewer and fewer paleopole are presented in publications with respect to classical geological, stratigraphic, or structural aspects, including those assigned to the topic "tectonic history of the Earth." And yet, paleomagnetism as a field of study and research of tectonic aspects is alive and well and manages to produce more journal articles and database than ever. Moreover, this is not all: several books have also seen the light in the last decade. One book we are able to highlight is the weighty monograph excellently predicted in 2017 by my co-author Trond Helge Torsvik from the University of Oslo and his colleague Robin Cocks for the Natural History Museum in London, entitled Earth History and Paleogeography, and published and marketed by Cambridge University Press.

The History of Remagnetization of Sedimentary Rocks: Deceptions, Developments and Discoveries

Rob van der Voo and Trond H. Torsvik

December 2012, Geological Society London Special Publications 371(1):23-53

Remagnetizations have been recognized ever since magnetizations in rocks were demonstrably shown to have been acquired at a much later time than the formation or deposition of the rocks themselves. There was mention of remagnetizations as early as the 1950s, and in the 1960s the concept was frequently hypothesized as an explanation for repetitions and loops in apparent polar wander paths. In this paper, remagnetization features and processes are organized by magnetic carrier: hematite, magnetite, Fe-sulphides and goethite. Selected case histories are presented which are chosen in order to reveal important diagnostics, although many origins of remagnetizations are still obscure or incompletely known.

New Concepts in Nanoscience: New Kinds of Materials opening the Way to New Technologies

by Herbert Gleiter, Member EUAS

Short Biography

Professional Career

Since 2015 ***Senior Fellow*** *(jointly with the Nobel and Fields Medal Laureates Haroche, Lehn and Small) of the Institute of Advanced Studies,* ***City University of Hong Kong.***

Since 2012 ***Founding Director*** *of the* ***Herbert Gleiter Institute of Nanoscience*** *of* ***Nanjing University*** *of Science and Technology, Nanjing, P.R.China*

Since 2006 ***Institute Professor*** *and* ***Distinguished Fellow*** *of the* ***Institute of Nanotechnology****, Karlsruhe Institute of Technology (KIT), Germany*

2007 - 2010 ***Distinguished Professor, Arizona State University****, Phoenix, USA*

2005 ***Distinguished Scholar*** *of the* ***Korean Research Foundation,*** *Seoul, Korea*

2004 - 2007 ***Kuang-pui Chair Professor, Zhejiang University****, Hangzhou, PR China*

1998 - 2004 ***Director*** *of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

1998 ***Founding Director*** *(jointly with Profs. J M Lehn and D. Fenske) of the* ***Institute of Nanotechnology****, Research Center Karlsruhe, Germany*

1994 - 1998 ***Member*** *of the* ***Executive Board*** *of the* ***Research Center Karlsruhe****, Germany*

1987 - 1994 ***Founding Director*** *of the* ***Institute*** *of* ***New Materials****, Saarbruecken, Germany*

1982 *Call to the* ***Federal Institute of Technology (ETH****) Zurich, Switzerland*

1980 *Call to the* ***University of Hamburg****-Harburg, Germany*

1973 -1994 ***Professor/Director*** *of the* ***Institute*** *of* ***Material Science****, University of the Saarland, Germany*

1972 ***Professo****r, Institute of Materials Science,* ***University Bochum****, Germany*

1971 ***Visiting Scientist*** *of the* ***Massachusetts Institute of Technology (MIT),*** *Cambridge, USA*

1970 *D. Sc. (Habilitation)* ***in Material Science*** *at the University of Bochum, Germany*

1966 - 1969 ***Research Fellow*** *at* ***Harvard University*** *Cambridge, USA*

1966 *Ph.D. in* ***Physics*** *at the Technical University of Stuttgart, Germany*

1959-1965 *Student of* ***Mechanical Engineering and Physics*** *at the Technical University of Stuttgart*

Honours and Awards (selection)

2018 ***Jan Czochralski Medal and Award,*** *Polish Academy of Science, Warsaw University,*

2016 ***Friendship Award*** *and* ***Medal of Merit*** *of Chinese Government, Jianzu, China*

2015 ***Cothenius Medal*** *of the German National Academy of Sciences - Leopoldina*

2015 ***Honorary Doctor*** *of the City University of Hong Kong*

2014 ***2014 Distinguished Lecturer****, University of Hong Kong*

2012 ***Zijin Chair Professor Award*** *of the Herbert Gleiter Institute of Nanoscience of the Nanjing University of Science and Technology, Nanjing, China*

2012 ***Nanomaterials Award 2012***

2012 ***Edward DeMille Campbell Award****, American Society for Metals (ASM)*

2009 ***R.F. Mehl Award*** *of the Minerals, Metals, Materials Society, USA*

2009 ***Blaise Pascal Medal*** *of the European Academy of Sciences, Belgium*

2009 ***NANO Today Award*** *of the Agency for Science, Technology Research, Singapore*

2008 ***Honorary Doctor*** *of the University of Muenster, Germany*

2008 ***Honorary Doctor*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

2008 ***Achievement Award NANOSPD*** *Int. Steering Committee*

2008 ***Staudinger-Durrer Award*** *of the Federal Institute of Technology (ETH) Zurich, Switzerland*

2008 ***Honorary Member*** *of the German Materials Society DGM*

2008 ***Von Hippel Award*** *of the Materials Research Society, USA*

2007 ***Gold Medal*** *of Acta Materialia*

2006 ***Humboldt Medal*** *of the Alexander von Humboldt Foundation, Germany*

2005 ***Distinguished Scholar*** *of the Korean Research Foundation*
2004 ***Honorary Professor*** *of Lanzhou University, PR China*
2004 ***H. Lee Lecture Award*** *of Chinese Academy of Science*
2004 ***Honorary Professor*** *at Zhejiang University, Hangzhou, PR China*
2003 ***Nanomaterials Award*** *of the Deutsche Bank, Germany*
2002 ***Honorary Doctor*** *of the Technical University of Darmstadt, Germany*
2000 ***Van Horn Award*** *of Case Western University Cleveland, USA*
1999 ***Werner Heisenberg Medal*** *of the Alexander von Humboldt Foundation, Germany*
1998 ***Heyn Medal*** *of the German Society for Materials Science*
1995 ***Gold Medal*** *of the Federation of European Material Societies (FEMS), Belgium*
1993 ***Vinci of Excellence Award*** *of the Hennessy-Vuitton Foundation, France*
1993 ***Max-Planck-Research Prize*** *of the Humboldt Foundation and the Max Planck-Society, Germany*
1992 ***Member of the President's Council*** *of the University of Illinois, USA*
1992 ***TMS Lecture Award*** *of the US Minerals, Metals and Materials Society*
1991 ***Order of Merit*** *of Saarland, Germany*
1988 ***Leibniz Prize*** *of the German National Science Foundation (DFG)*
1984 ***Alcoa Prize*** *of the Alcoa Foundation, USA*
1979 ***Karl-Schurz Award*** *of the University of Wisconsin, USA*
1972 ***Masing Prize*** *of the German Society for Metals*

Memberships in National Academies

1998 Member of the ***German National Academy of Sciences*** *– Leopoldia, Germany,*
2004 Member of the ***US National Academy of Engineering***
2004 Member of the ***American Academy of Arts and Sciences***
2006 Member of the ***Indian National Academy of Engineering***
2007-12 ***Vice President*** *of the* ***German National Academy*** *of Sciences*
2009 Member of the ***European Academy of Sciences***
2009 Member of the ***Indian Academy of Sciences***
2011 Member of the ***Indian Science Academy***
2014 Member of the ***Academia Europaea***
2014 Member of the ***European Academy of Sciences and Arts***
2015 Member of the ***EU Academy*** *of* ***Sciences***
2016 Member of the ***US National Academy of Inventors***

Founding of a New Research Institute

*Founding of the "****Herbert Gleiter Institute of Nanoscience****" in 2012 at Nanjing University of Science and Technology. This Institute is planned to have a size and a structure of a Max Planck Institute in Germany.*

Today's technologies are based primarily on utilizing crystalline materials (such as metals, semiconductors or crystalline ceramics) with crystal sizes in the order of a few micrometers or more.

The way to new kinds of materials was opened in 1980 by reducing the crystal sizes of crystalline materials to a few nanometers resulting in so called Nano-crystalline materials. They consist (by comparable volume fractions) of nanometer-sized crystalline regions (of identical or different chemical compositions) connected by (nanometer-wide) inter-crystalline interfaces. Due to the new atomic arrangements in these inter-crystalline interfaces, Nano-crystalline materials have new atomic as well as new electronic structures and hence new properties. So far, this development resulted in more than 100 000 publications that were retrieved in this field by the Web of Science up to 2019 and in commercial products of values of more than 2 billion US$.

In 1989 a new kind of nano-structured non-crystalline materials, so called Nano-glasses, were proposed. They consist of nanometer-sized glassy regions (of identical

or different chemical compositions) connected by (nanometer-wide) interfacial non-crystalline regions with atomic and electronic structures that do not exist in melt-cooled glasses. Due to their new atomic/electronic structures, the properties of Nano-glass differ from the properties of the corresponding, chemically identical melt-quenched glasses. For example, their ductility, their biocompatibility, their catalytic and ferromagnetic properties are changed by up to several orders of magnitude. Moreover, they permit the alloying of components e.g. ionic materials (e.g. SiO) and metallic materials (e.g. PdSi glasses) that are immiscible in the crystalline state as well as in melt-quenched glasses . The properties of Nano-glasses may be controlled – just like in today's technologically used crystalline materials - by varying the sizes and/or chemical compositions of the glassy clusters which opens the perspective of a new technology age - a "Glass age".

Another group of nano-structured materials with tunable properties are nano-porous metals with electrolyte filled pores. By applying an external voltage between the electrolyte and the nano-porous metal, their properties e.g. their superconductivity, magnetic moment, electric resistivity may be varied dramatically. For example, artificial muscles have been produced by means of carbon nanotube tissues or nano-porous metals.

These Studies are performed at present at the two Institutes mentioned at the beginning of this article.

Starting in 2022 the Chinese Academy of Science will open a new research center at Sheyang (PR China) the Herbert Gleiter Internatioal Laboratory (HGIL).A photo of this HGIL is attached at the end of this article

References

Nanocrystalline materials
H. Gleiter
Progress in Materials Science **33** (1989) 223-315
Nanoglasses
H. Gleiter
Small **22** (2o16) 2225-2233
Nanostructured solids – From nano-glasses to quantum transistors
H. Gleiter, Th. Schimmel, H. Hahn
Nano Today **9** (2014) 17 - 68

Geo-Surveying and Mapping of Environmental Dynamics Using Remote Sensing Approaches

by Manfred F. Buchroithner EUAS

Short Biography

*Manfred Ferdinand Buchroithner (*17-12-1950) studied Geology & Palaeontology at the University of Graz/Austria and both Remote Sensing and Cartography at ITC/Netherlands. He obtained his PhD in 1977 in Graz. In 1982 he went as Fulbright Scholar to the USA (Fort Worth/Texas, Boulder/Colorado and Stanford University/California). During the following years at the Institute for Cartography of the Austrian Academy of Sciences in Vienna and as Director of the Joanneum Research Institute of Digital Image Processing and Computer Graphics in Graz he spent several months of postdoctoral research at the Finnish National Research Center/VTT in Espoo near Helsinki and at the Jet Propulsion Laboratory/JPL of NASA in Pasadena. In 1985 he obtained his habilitation (venia legendi) for both General Geology and Remote Sensing. From 1992 to 2016 he was Full Professor, holding the Chair of Cartography at TU Dresden, Germany. Subsequently he held the position of a Senior Professor for two years. M. F. Buchroithner led many expeditions to high mountain regions in the Andes, Alps, Balkan mountain ranges, Kilimanjaro Massif, Altai mountains, most of the regions of High Asia (Tian Shan, Pamir, Hindu Kush, Karakorum, Himalaya, Tibet incl. Nyenchen Tanglha Mountains and Kailash) and to Borneo/Malaysia. He spent semesters as Invited Professor at the Universities of Munich/Germany, Salzburg/Austria (twice), Bergamo/Italy, COMSATS/Islamabad, and the École Nationale Superieur des Mines des Paris in Sophia Antipolis/France and also gave invited guest lectures at various Chinese universities. He supervised and successfully graduated more than 50 doctoral students. Buchroithner both authored and edited several books on cartographic, GIT and remote sensing issues and has more than 475 publications incl. maps and several educational films to his credit.*
He holds international patents in 3D cartography, is member of several learned societies and obtained a series of national and international scientific awards, i.a. the Friedrich Hopfner Medal (A) and the Denny Medal (UK).

Research Activities

Buchroithner, M. F. & Gaisecker, Th. (2020): Ice Surface Changes in Eisriesenwelt (Salzburg, Austria) Based on LIDAR Measurements between 2017 and 2020. Die Höhle , 71. Jg., 1–4/2020: 62 -70. Vienna, Austria.

Abstract

Based on highly accurate laser detection and ranging (LIDAR) surveys in the show cave part of Eisriesenwelt in 2017, 2019 and 2020, areal and mass-related comparisons of the ice cover were carried out. The results show that within this three-year period the total ice surface of about 11,100 m2 remained nearly constant and a slight increase in ice volume occurred. Detailed three-dimensional visualisations of the dynamics of the ice surface within the study period show the following results.
The most recent LIDAR surveying campaign in the Eisriesenwelt end of April 2020

resulted in a total ice surface of roughly 10,100 m². Compared to 2017, an area of 2660 m² remained more or less constant, i.e. the average ice thickness changed by less than 3 cm. Approximately 3860 m² showed an ice decrease of up to 30 cm (locally even more), whereas for about 3500 m² an increase of the same amount was measured. The comparison of the overall mass balance of the Eisriesenwelt between the two survey campaigns (April 2017 and April 2020) yielded an ice increase of 59 m³ (Fig. 9). This has to be seen in relation to the total ice mass calculated by Kaidong (2018) based on ground-penetrating radar measurements taken in April 2017, i.e. approximately 63,300 m³.
The flat area of the cave shows minor ice changes with smaller maximum decreases and increases (Fig. 8, 9). We assume that the reason is the flat topography with just a few small water inflows. The mass balance of this flat area yielded an ice decrease of 21 m³. The rearmost ice- filled part of the cave, *Eispalast*, is also a flat area, but interestingly it shows a strong ice growth of 88 m³ (Fig. 8, 9).
To sum up, the ice volume in Eisriesenwelt has increased slightly even in recent years of increased global warming. Future LIDAR surveys will show whether this is a multi-annual trend, providing important highly resolved data for a better understanding of the long-term ice mass balance in this cave.

Twisa, S., Kazumba, S., Kurian, M. & Buchroithner, M.F. (2020): Evaluating and Predicting the Effects of Land Use Changes on Hydrology in Wami River Basin, Tanzania. Hydrology, 2020, 7, 17: 18 pp. DOI: 10.3390/hydrology 7010017.

Abstract

Understanding the variation in the hydrological response of a basin associated with land use changes is essential for developing management strategies for water resources. The impact of hydrological changes caused by expected land use changes may be severe for the Wami River System, given its role as a crucial area for water, providing food and livelihoods. The objective of this study is to examine the influence of land use changes on various elements of the hydrological processes of the basin. Hybrid classification, which includes unsupervised and supervised classification techniques, is used to process the images (2000 and 2016), while CA–Markov chain analysis is used to forecast and simulate the 2032 land use state. In the current study, a combined approach —including a Soil and Water Assessment Tool (SWAT) model and Partial Least Squares Regression (PLSR) — is used to explore the influences of individual land use classes on fluctuations in the hydrological components. From the study, it is evident that land use has changed across the basin since 2000 (which is expected to continue in 2032), as well as that the hydrological effects caused by land use changes were observed. It has been found that the major land use changes that affected hydrology components in the basin were expansion of cultivation land, built-up area and grassland, and decline in natural forests and woodland during the study period. These findings provide baseline information for decision-makers and stakeholders concerning land and water resources for better planning and management decisions in the basin resources' use.

Twisa, S., Mwabumba, M., Kurian, M. & Buchroithner, M.F. (2020): Impact of Land-Use/Land-Cover Change on Drinking Water Ecosystem Services in Wami River Basin, Tanzania. Resources, 2020, 9, 37: 18 pp. DOI: 10.3390/resources9040037.

Abstract

Land-use/land-cover changes are considered the dominant form of anthropogenic pressure on the environment, causing changes in ecosystem service patterns and affecting water supply services. Using the spatial econometric technique, we analysed the impact of land-use/land-cover change on water ecosystem services for domestic use upstream and downstream of the Wami River Basin. The results in terms of land-use/land-cover classes during the study period (2011–2016) indicate that cultivated land showed maximum positive changes in both sub-catchments, while bushland and woodland showed maximum negative changes upstream and downstream. The results showed that bushland, woodland, cultivated land, and grassland were significantly correlated with water point characteristics in both sub-catchments. For functionality characteristics, a significant effect was observed in bushland and grassland upstream and downstream, respectively, while sufficient water was found in woodland upstream and grassland downstream. Moreover, bushland was observed to have a significant number of water points with poor quality of water upstream, and a substantial number of water points with good quality of water were found in grassland downstream. We found that all measured land-use/land-cover changes and water point characteristic correlations were statistically significant; therefore, we concluded that land-use/land-cover change affects the water ecosystem in the basin. These results could facilitate decision-making and development of related policies and might support finding sustainable strategies for water ecosystem services for domestic use.

Shirvani, Z., Abdi, O. & Buchroithner M.F. (2020): A New Analysis Approach for Long-Term Variations of Hyrcanian Forest Loss, Fragmentation and Degradation 1966-2016 Resulting from Road-Network Expansion Using Landsat Time-Series and Object-Based Image Analysis. A Case Study in NE Iran. Land Degradation and Development, 2019: 39 pp. DOI: 10.1002/ldr.3530.

Abstract

Despite facilitating transport by low-volume roads for multiple purposes, these roads also open corridors to the remote pristine forests and accelerate forest dynamics with deleterious consequences to the forest functionalities and indigenous inhabitants. We assessed the spatial variations of Hyrcanian forest loss, fragmentation, and degradation resulting from the expansion of rural, logging, and mine roads between 1966 and 2016 in northeast Iran. Various data were employed to generate a precise road network; the density of road segments was weighted on the basis of their carrying capacity during 1966–1986, 1986–2000, and 2000–2016. Three dimensions of forest changes were retrieved using the Landsat time-series and object-based image analysis. The spatial patterns of high rates of forest changes were clustered using spatial autocorrelation indicators. The spatial regression models were carried out to explore relationships between forest change and road expansion. The results showed that rural roads were upgraded but forest and mine roads remarkably expanded in recent decades. The spatial variations of forest-dynamic patterns have been changing from forest loss (1966–2000) to forest fragmentation and degradation (1986–2016). The high density of rural roads was significant on the high rates of forest loss and fragmentation during 1966–2000, and the expansion of forest and mine roads significantly intensified the rates of fragmentation and degradation during 1986–2016. Our findings suggest for mitigating destructive schemes over Hyrcanian forests, developing either protected areas or joining unprotected forests to the reserved areas should be

prioritized.

Bayramov, E., Manfred Buchroithner, M.F. & Kada, M. (2020): Quantitative Assessment of Ground Deformations for the Risk Management of Petroleum and Gas Pipelines Using Radar Interferometry. Geomatics, Natural Hazards and Risk, 11, 1: 2540 - 2568, DOI: 10.1080/19475705.2020.1853611.

Abstract

The primary objective of these studies was to quantitatively assess the ground deformation velocities and rates and their natural and man-made controlling factors as the potential risks along the seismically active 70 km section of buried Baku-Tbilisi-Ceyhan Oil, South Caucasus Gas, Western Route Oil and South Caucasus Pipeline Expansion Gas pipelines in Azerbaijan using Persistent Scatterer Interferometric Synthetic Aperture Radar (PS-InSAR) technique.

PS-InSAR analysis showed that the continuous subsidence was prevailing in the kilometer range of 13-70 of pipelines crossing two active seismic faults. The ground uplift deformations were observed in the pipeline kilometer range of 0-13. The minimum and maximum vertical ground movement velocities were observed to be −21.3 mm/y and 14.1 mm/y along 70 km section of pipelines with 250 m buffer zone. Both of these sites were observed at the range of seismic faults. The spatial distribution of sites with ground deformation velocity less than −15 mm/y and more than 15 mm/y was diverse and random all along 70 km of pipelines without any cumulative spatial patterns.

Based on the lower mean, variation and standard deviation of pixel values, the seismic fault in the kilometer range of 21-31 revealed its higher vulnerability to subsidence processes rather than the Seismic Fault in the kilometer range of 46-54. The ground deformation velocities within the range of Seismic Fault KP21-31 revealed the minimum and maximum values of −19.74 mm/y and 14.1 mm/y, respectively whereas at the Seismic Fault KP46-54, the minimum and maximum values were −17.07 mm/y and 9.29 mm/y, respectively. An encouraging level of agreement with the regression coefficients of 0.92 and 0.96 for known subsiding sites at KP28 + 500 and KP52 + 750 and 0.97 and 0.96 for known uplifting sites at KP04 + 900 and KP35 + 050 respectively was observed between the high-precision GPS and PS-InSAR measurements.

The diverse spatial distribution and variation of ground movement processes along pipelines demonstrated that general geological and geotechnical understanding of the study area is not sufficient to find and mitigate all the critical sites of subsidence and uplifts for the pipeline operators. The prediction of the potential subsidence or uplift locations based on the field visual verifications holds a lot of uncertainties without broad and detailed scale airborne and satellite space observation technologies. The justification of the budget for the geotechnical maintenance activities along long-range oil and gas pipelines requires sophisticated prioritization and planning of the remediation sites and clear quantitative and qualitative risk assessment proving the activeness of these sites and effectiveness of the remediation measures. This means that the PS-InSAR – based approach outlined in this paper is a significant improvement over current ground-based monitoring practices or can significantly contribute them in the initial phase of risk assessment and prioritization.

Ji, M., Liu, L., Zhang, R. & Buchroithner, M.F. (2020): Discrimination of Earthquake-Induced Building Destruction from Space Using a Pretrained CNN Model. Special Issue of Advanced Remote Sensing Technologies for Disaster Monitoring. ***Applied Science,*** **2020,** ***10*****(2), 602: 12 pp.**
DOI: https://doi.org/10.3390/app10020602.

Abstract

The building is an indispensable part of human life which provides a place for people to live, study, work, and engage in various cultural and social activities. People are exposed to earthquakes, and damaged buildings caused by earthquakes are one of the main threats. It is essential to retrieve the detailed information of affected buildings after earthquakes. Very high-resolution satellite imagery plays a key role in retrieving building damage information since it captures imagery quickly and effectively after the disaster. In this paper, the pretrained Visual Geometry Group (VGG)Net model was applied for identifying collapsed buildings induced by the 2010 Haiti earthquake using pre- and post-event remotely sensed space imagery, and the fine-tuned pretrained VGGNet model was compared with the VGGNet model trained from scratch. The effects of dataset augmentation and freezing different intermediate layers were also explored. The experimental results demonstrated that the fine-tuned VGGNet model outperformed the VGGNet model trained from scratch with increasing overall accuracy (OA) from 83.38% to 85.19% and Kappa from 60.69% to 67.14%. By taking advantage of dataset augmentation, OA and Kappa went up to 88.83% and 75.33% respectively, and the collapsed buildings were better recognized with a larger producer accuracy of 86.31%. The present study showed the potential of using the pretrained Convolutional Neural Network (CNN) model to identify collapsed buildings caused by earthquakes using very high-resolution satellite imagery.

Some New Progress on Structural Safety and Control

by Hong-Nan Li, Member EUAS

Short Biography

Dr. Hong-Nan Li received his bachelor's degree from Shenyang Jianzhu University in 1982, his master's degree and PhD from the China Earthquake Administration in 1987 and 1990, respectively. He had conducted his postdoctoral research at Virginia Polytechnic Institute and State University from 1992-1994. He is the Distinguished Professor of School of Civil Engineering at Dalian University of Technology (DUT), China. He is the founding director of the Research Center for Structural Health Monitoring and Control at DUT.

He is a Fellow of American Society of Civil Engineers (ASCE). His research interests are primarily in safety and security of civil infrastructure systems, focusing on development of innovative and interdisciplinary science and technology for sensors, health monitoring, damage assessment, structural control and disaster prevention. He is the author/co-author of 8 books and more than 400 refereed journal papers including more than 300 international journals. He is also an inventor or co-inventor of 67 invention patents and 8 computer software certificates. He has delivered over 80 keynote and invited lecture at international conferences and universities in different countries.

He edited the first ever standard in the area of SHM in China "Design Standard for Structural Health Monitoring Systems (CECS 333: 2012)" and other 15 standards. His related achievements have been applied to more than 70 major infrastructures, such as the Zhoushan Transmission Tower (The World's the Tallest Transmission Tower), Dalian gymnasium (The World's Largest Span Suspended Dome Structure), the long span suspension dome structure NB35-2 (Ultra Large Offshore Oil Platform), Shenyang Boguan bridge (Complicated Long-Span Arch Bridge), Dalian World Trade Center. He received various prizes in recognition of his innovative achievements in research, such as played a leading role in the 2015 National Technology Invention Award, 2010 & 2007 National Science and Technology Progress Awards, and more than 10 provincial Science & Technology awards in China. He was also awarded as the "Outstanding Technical Contribution Award" by ASCE Aerospace Division (2014)

With a long-term commitment to serving society, He is currently the Editor-in-Chief of Structural Monitoring and Maintenance, An international Journal, Associate Editor of Journal of Aerospace Engineering-ASCE and an editorial board member of more than 30 other journals. He also has held many extensive academic and professional leadership positions related to SHM: vice chair of the Advanced Materials and Structures committee & vice chair Dynamics and Controls Committee, American Society of Civil Engineers (ASCE); vice chair of China Panel, International Association for Structural Control and Monitoring (IASHM); council member of The International Society for Structural Health Monitoring of Intelligent Infrastructure (ISHMII), vice chair of the board for the Society of Structural Anti-Seismic, a branch of the Chinese Society of Vibration Engineering, etc.

He was elected as a Fellow of ASCE in 2017. He was honored as Distinguished Professor in Cheung Kong Scholars Program by Ministry of Education of China, National Science Foundation for Distinguished Young Scholars of China (NSFC), National Young and Middle-aged Expert with Outstanding Contributions by Ministry of Human Resources and Social Security of China, State

Department experts enjoying special government allowances by State Council of China, etc.
Dr. Li promoted the education of undergraduate students and graduate students in Civil Engineering. He has supervised more than 54 Ph.D. students and 70 Master students. Some thesis from his students were awarded for the provincial excellent theses.

Some New Progress on Research Activities

1. Hysteretic model considering dynamic effect and deterioration for seismic performance analysis of reinforced concrete structures

An innovative approach is developed to consider the impact of dynamic effect and deterioration on the seismic performance analysis of reinforced concrete frame structures. Firstly, based on the established dynamic loading test database of RC column specimens, the predicted models of dynamic modified coefficients are constructed to take into account the impacts of dynamic effect on the yielding and ultimate strength, effective stiffness and ductility coefficient of RC columns. Secondly, a damage index-based hysteretic model is proposed which is capable of reflecting both cyclic and in-cycle performance degradation of RC columns under cyclic dynamic loading. Finally, by employing the dynamic modified coefficients into the restoring force model, the influences of dynamic effect and deterioration on the seismic behaviors of a RC frame structure with its prototype model suffering from severe damage in the Yushu earthquake in China are comprehensively investigated. The superiority of the proposed approach over the traditional method lies in that both the advantage and disadvantage aspects of dynamic effect can be considered. Moreover, the effectiveness and accuracy of the developed models are verified with the dynamic loading experimental observations. By comparing the numerical results of seismic responses between the rate-independent and rate-dependent models, it is found that the dynamic effect can exert dual influences on the structural seismic performance. For the frame models subjected to earthquakes with small intensities, the displacement response and damage degree can be reduced due to the strength and stiffness enhancement of structural members. As for the frame models undergoing serious failure under the large intensity excitations, the structural damage is aggravated and the failure mechanism may be affected because of the decreased ductility and intensified deterioration caused by the dynamic effect. To provide a more reliable seismic performance assessment of RC structures, it is suggested that the combined influences of dynamic effect and deterioration should be given an adequate consideration in the further research works.

2. Experimental and analytical investigations on new viscoelastic damped joints for seismic mitigation of structures with precast shear walls

Precast concrete wall has become a crucial part in the architectural industrialization, which is in line with the development trend of the building industry. Based on the analysis of relations between the deformation and the energy distribution of the precast concrete walls under major earthquakes, this investigation proposes the idea of a novel viscoelastic damped joint (VDJ) to create the vertical connection between two precast walls. By amplifying the displacements and velocities of the joint, the energy dissipating properties of damping materials can be fully used. The VDJ is suitable for improving the damping efficiency in the stiff shear wall structural systems. Performance tests were performed to study the mechanical properties of the damped joint. And then, a simplified analytical model of the VDJ with different parameters under various deformations and frequencies is presented. The numerical simulation results indicate that the simplified model is capable of capturing the main features of the VDJ. Furthermore, the analytical models on wall to wall connections were set up and incorporated into 2D numerical models. To better understand the damping performances of the VDJ, three models connected by emulating cast-in situ joints, precast hinged joints and viscoelastic-damped joints were prepared by analyzing the time history of the overall structural response. Results show that the VDJs are effective in attenuating seismic response of the precast walls. They worked in the dissipation approximately 90% of input earthquake energy. The highly efficient damped joints also reduce inter-story displacements and upgrade the structural performance of buildings during seismic excitation.

3. Experimental characterization and theoretical modeling of a gear driven rotation-amplified viscoelastic shear damper

Seismic damage of frame structures is normally concentrated in the area of beam-column joints, the failure of which not only easily leads to global destruction and collapse of the structure, but also to the difficulties in repairing after the earthquake. However, the relative angle deformation between the beam and column is small for the concrete structures subjected to dynamic loads (e.g. earthquake and wind), and the most metallic dampers installed here are little effective. To overcome this problem, this paper presents an innovative gear driven rotation-amplified viscoelastic shear damper (GDRAD) to reduce the seismic shift responses of beam-column connections in frame structures. The damper can amplify the angular displacement according to actual needs and fully exploit the energy dissipation capacity of viscoelastic materials. First, the design philosophy, basic construction, working mechanism and outstanding features of this damper are introduced. Then, low cyclic loading tests of the fabricated GDRAD are conducted to study the influence of shear strain amplitude and loading frequency on the damper’s mechanical properties, and the results show that this damper has stable hysteretic and great anti-fatigue

performances. Finally, based on material characteristic tests and geometric relationships of the damper components, a modified theoretical model that can reproduce the hysteretic responses of the GDRAD at different loading conditions is proposed.

4. A re-centering deformation-amplified SMA damper for mitigating seismic response of structures

A re-centering deformation-amplified shape memory alloy damper (RDMSD) was presented to reduce the responses of civil structures under earthquake motions. The damper is with the mechanism of deformation amplification and fully exploit the energy dissipation capacity of superelastic SMA materials. The cycling tests of fabricated RDMSD were conducted to study the influence of deflection amplitude and loading rate on the damper's mechanical properties. Additionally, a theoretical model of the RDMSD is proposed to precisely simulate the hysteretic characteristics of the damper. The nonlinear time history analysis was performed on a six-story steel frame without dampers and with dampers including the amplification and no-amplification functions. The results for the numerical analysis showed that the proposed RDMSD not only can effectively mitigate the displacement, acceleration and interstory drift responses due to its efficient energy dissipation capacity, but also can provide superior re-centering by amplifying the relative deflection for building structures subjected to strong earthquakes. Thus, in practical applications, the recommended range for the displacement amplification coefficient of the damper is 2.0–3.0.

5. Interactive multi-objective optimization involving engineering preference for life-cycle seismic design of bridges

Considering the future seismic capacity and life-cycle cost, the life-cycle seismic design of bridges is formulated as an interactive multi-objective optimization and decision-making problem. Specifically, the preference information based on the theoretical analysis and engineering judgement is embedded in the optimization procedure. The posteriori evolutionary multi-objective optimization (EMO) algorithm (non-preference) and the preference-based interactive EMO algorithm are both applied to the seismic design of an RC pier with two, three and four objectives, namely, flexural strength coefficient, shear strength coefficient, reliability index of drift and life-cycle cost coefficient. Based on a reasonable displacement ductility, the safety preference information is used to construct a value function after every few optimization runs, progressively directing the search of the EMO algorithm to more preferred solutions. By comparing the results of both algorithms, it is found that when there are more than three objectives, it is difficult for the non-

preference optimization to converge with the global Pareto frontier, resulting in a local optimal solution as the final design. The combination of preference structure and multi-objective optimization is able to effectively avoid the challenges of global search and purposefully converge with the most preferred design.

6. A novel friction damped joint of precast concrete wall and its performance when considering damage-plasticity control

This study presents the development of a novel friction damped joint (FDJ) which can be installed between two precast concrete walls as a type of vertical connector. The specially designed internal mechanism of the proposed FDJ can amplify the vertical slip displacement between the precast concrete walls whilst dissipating energy at the same time. Meanwhile, the FDJ can provide enough lateral strength and stiffness to resist the vertical slips due to the wind forces and small earthquakes. After experimental and analytical studies on the FDJ parameters, including the loading frequency, displacement amplitude, friction interface and normal force, the energy dissipated by the proposed FDJ is found to be independent of the excitation frequency. Then, a simplified numerical model of the FDJ with different parameters that relate to the displacements, the normal force and the friction interface is presented. The simulation results indicate that the simplified numerical model can capture the main features of the FDJ. To further illustrate the advantage of the FDJ when considering damage-plasticity control, simulated precast walls with different joints are analyzed under the lateral loading. The results show that the FDJ can consume a significant amount of energy, thus protecting the precast walls from damage. The FDJ plays a great role in reducing the plastic damage of the main structure.

Improvements in Artificial Photosynthesis - Photochemical reduction of Carbon Dioxide

by Björn Åkermark, Member EUAS

Short Biography

Name:	*Björn Åkermark*
Date of birth:	*1933-12-19*
Nationality:	*Swedish*
Languages:	*Swedish, English, German, French, Italian*
1967	*Doctor of Technology, Royal Institute of Technology (KTH), Stockholm*
1957	*M.Sc. in Chemical Engineering, KTH, Stockholm*
1953	*Studies at Colorado College, Colorado Springs, USA*
Position Held	
1999–present	*Guest professor and research leader at Stockholm University (SU),*
1999	*Professor emeritus, KTH*
1980-1998	*Full professor, KTH*
1994-1997	*Dean of undergraduate studies, Faculty of Chemistry and Chemical Engineering, KTH*
1985–1998	*Associate professor, Colorado State University, Fort Collins, USA*
1987	*Visiting professor, Aix-Marseille University, Marseille, France*
1984–1987	*Dean of undergraduate studies, Faculty of Chemistry and Chemical Engineering, KTH*
1977–1978	*Visiting scholar, Stanford University, Stanford, USA*
1972–1980	*Associate professor, KTH*
1967–1972	*Assistant professor, KTH*
1967–1968	*Visiting scholar, Stanford University, Stanford, USA*
1963–1972	*Lecturer in Organic Chemistry, KTH*
Professional Activity beside Teaching and Research	
1987–1990	*Member of the Reference Group for Research and Combustion, Swedish Energy Agency*
1986–1989	*Member of the Committee for Mercury in the Environment, Swedish Environmental Agency*
1985–1994	*Member of the research board, Nobel Industries*
1985–1988	*Member of the Committee for Toxicology and Health Effects, Swedish Environmental Agency*
1981–1986	*Member of the Board for the STU-program Applied Organic Synthesis*
1979–1985	*Member of the Board of the Foundation for Industrial Electrochemistry*
1976	*International expert in Italy in connection with the Seveso accident*
1971–1994	*Consultant, Nobel Industries*
Awards	
2009	*Ulla and Stig Holmquists prize, Uppsala University*
2009	*The Bror Holmberg Medal, The Swedish Chemical Society*
1991	*KTH Prize for Excellence in Teaching, KTH*
1978	*The Arrhenius Medal, Swedish Chemical Society*
1977	*The Zorn Fellowship, Sweden-America Foundation*
1976	*Letterstedt Award, Royal Swedish Academy of Sciences*

Current Memberships
Swedish Chemical Society, American Chemical Society, World Academy of Art and Science, EU Academy of Sciences.
Publications
Author of 299 publications in international journals, of which 144 were published since retirement 1998; h-factor 68 according to Google Scholar.

Bjorn Akermark became Dr of Technology at the Royal Institute of Technology in Stockholm and assistant professor of Organic Chemistry in 1967.
During the dissertation work, which dealt with the structure and synthesis of a few lichen compounds,[1] he realized that synthesis of organic compounds such as fine chemicals and pharmaceuticals were general prepared in a very wasteful way, despite the fact that there were a few large scale processes, such as the Haber-Bosch conversion of molecular nitrogen into ammonia and the very recent production of acetaldehyde from ethane (the Wacker process) which were selective catalytic processes. He realized the necessity to use catalysts with similar function as the natural enzymes, and simple reactants such as oxygen and hydrogen. In the synthetic work with lichen compounds, he therefore started to use less conventional ways of forming C-C bonds, such as the Ullman copper catalyzed coupling of aryls to biaryls[2] and the Kolbe electrolytic coupling of alkyls to dialkyls.[3] He also worked with mercury promoted formation of carbenes to synthesize □ □-lactams.[4]

After the dissertation he went to Stanford University as visiting scholar 1967-1968, working on nitrogen fixation with professor Eugene vanTamelen. He developed an early electrolytic process for reduction of nitrogen to ammonia, using titanium catalysis.[5] Back in Sweden, he improved the reaction by using low melting mixed chlorides as solvent.[5] During the year at Stanford, thanks to the interaction with vanTamelen and professors Henry Taube and James Collman, he began to get a grip on the then magic world of transition metal catalysis. Together with an industrial college, professor Kjell Sjöberg, he was able to introduce homogenous catalysis in Sweden in the form of palladium promoted amination of simple alkenes.[7] As part of this work, he was able to show later that the related addition of water to alkenes in the Wacker process proceeded in a trans fashion.[8] Via the work with amination he became involved in palladium catalyzed nucleophilic substitution of allylic acetate by amines and other nucleophiles[9] and palladium promoted conversion of alkenes into allyl acetates.[10] In extensive studies, he clarified the mechanism of these reactions,[11] and the influence of N,P ligands on their selectivity and how chirality could be introduced.[12,13] He also worked with insertion into alkenes as a typical cis addition and could show that steric factors are important. Thus addition of nickel hydride to alkenes, a standard cis addition, in fact proceeded trans when 1,5-cyclooctadiene was used as alkene.[14] He also participated in an early quantum chemical study of the insertion reaction on ethene.[15] The interest in the insertion reaction later led to studies of the palladium catalyzed Heck reaction, where early work in cooperation with Nobel Industries and Astra (Anders Hallberg) led to attempts to prepare the beta-blocker Metoprolol by the Heck reaction. It also led to later studies of ways to direct the addition of palladium aryls to styrenes.[16]

Åkermarks early interest in C-C coupling led to further studies of both alkyl and aryl coupling. He was able to show that reductive aryl coupling via diarylnickel(II) could be induced by electrolytic oxidation of the initial Ni(II) to Ni(III).[17] He also participated in a theoretical study of this type of reductive elimination.[18]

The studies of allylic C-H activation, combined with the interest in C-C coupling, led to work with palladium promoted coupling of aryls and Åkermark could show that palladium

promoted double C-H activation and coupling of diphenylether to dibenzofurane and diphenylamine to carbazol was possible.[19] He could later develop an efficient catalytic version of this reaction.[20]

During the first big energy crisis in 1973 Åkermark realized that it was up to him and his colleges to solve the energy problem. He therefore initiated studies aimed at artificial photosynthesis. He focused on photochemical reduction of carbon dioxide. Progress was sluggish and after great efforts, one paper was pubished, describing photochemical reduction of carbon dioxide all the way to methane, promoted by an iron-phenanthroline complex.[21] He left the area until 1989, when he as offered a grant from the Swedish Energy Research Council (now the Swedish Energy Agency) and initiated renewed studies of artificial photosynthesis together with a specialist on flash photolysis, professor Mats Almgren at Uppsala University. In 1995, two more colleges were added, professors Stenbjörn Styring and Sten-Eric Lindquist, and the Swedish Consortium for Artificial Photosynthesis was formed, now supported by the Wallenberg Foundation. The initial studies focused on the properties of photosensitizers related to (trisbipyridine)ruthenium(II). An interesting result of these early studies was that the positively chargd acceptor methylviologen could penetrate a micelle membrane via dispropornation of two methyl radicals formed by electron donation from excited Ru sensitizers to methylviologen and the neutral doubly reduced methylviologen.[22] Another interesting result was that the introduction of carboxylate into the bipyridine unit of (trisbipyridine) type Ru(II) complexes reduced the Ru(II) to Ru(III) redox potential remarkably.[23]

The crucial problem in mimicking natural photosynthesis to covert solar energy into fuel is to oxidize water to molecular oxygen, that is to collect the electrons required to reduce carbon dioxide to biomass, or in a simpler process, protons to molecular hydrogen, from water.

The work of the consortium focused on two areas, (1) studies of manganese complexes for water oxidation and (2) synthesis and properties of coupled sensitizer-manganese complexes, that could photochemically generate the desired electrons. A number of different mono and dinuclear manganese complexes were prepared.[24] However, neither these nor the majority of other reported complexes were able to oxidize water by stepwise 1-electron transfer as taking place in the natural photosynthesis. The major part of the work was concen-trated on complexes, where a manganese complex was coupled to a ruthenium sensitizer. A first example of electron transfer from manganese to an oxidized ruthenium sensitizer[25] was followed by a series of studies leading to a close model of PS II,[26] where a repeatedly generated oxidized ruthenium sensitizer was able to oxidize an attached dinuclear manganese complex in four steps, just as in the natural system. However, in the fourth oxidation step the manganese complex disintergrated, possibly giving a trace of water oxidation. Only in 2011, was Åkermark able to present a dinuclear manganese complex which did oxidize water by 1-electron transfer, albeit with low efficiency.[27]

In 2001 he also became interested in hydrogenase mimics as an attractive way to generate hydrogen by the electrons donated by the sensitizer to an acceptor. A model complex, with a hydrogenase model linked to a ruthenium sensitizer, was presented in 2003, but the redox potential of the excited sensitizer was insufficient to reduce protons with the hydrogenase catalyst.[28] A summary of early results was published 2005.[29] In 2008, the only example so far of photoinduced electron transfer from a sensitizer to a hydrogenase mimic was presented.[30]

From 2005 and onwards, he started working with ruthenium based water oxidation catalysts. Already in 1982 Thomas Meyer and his coworkers reported successful water

oxidation using a dimeric ruthenium bipyridine complex, the "Blue Dimer".[31] The efficiency was low and only in 2004-2005 the groups of Llobet and Thummel described Ru-complexes with higher efficiency.[32] Inspired by this work, and by our early study, which showed that introduction of carboxyl groups into bipyridine type ligands greatly decreased the redox potential of the complexes,[23] Åkermark and Licheng Sun prepared two complexes which were more efficient with turn over numbers up to 10000. [33] In continuation of this work, a number of new mono- and dinuclear catalysts were prepared. One complex is particularly interesting since quantum chemical calculations showed that of the two major mechanisms for water oxidation, the oxygen-oxygen coupling of two metal oxo groups, was greatly favoured over nucleophilic attack of water on one metal oxo group.[34] Lately, Åkermark has realized that time is running out and that although artificial photosynthesis may be the final elegant solution to the worlds energy problems, it requires very much more research. He has therefore recently began to study ways to improve the classical electrolytic splitting of water into hydrogen fuel and oxygen that can be used in combination with solar cells and wind mills. As a first step he and his coworkers have just prepared a new ruthenium complex[35] which shares the world record in rate, turn over rate ca 40000 s^{-1} , with a complex prepared by Llobet and coworkers.[36] This is at the level of the fastest known enzymes and offers great promise for the future.

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Impact Behavior of Unbonded Post-Tensioned Concrete Beams

by Thomas Kang, Member EUAS

Short Biography

Dr. Thomas Kang is a Professor of structural engineering in the Department of *Architecture & Architectural Engineering and the Director for Engineering Education Innovation Center & GECE (Global Education Center for Engineers) at Seoul National University (SNU), Korea, and served as a part of the Vice-Deans' group of the College of Engineering at SNU. Before that, he was an Assistant Professor in the School of Civil Engineering and Environmental Science at the University of Oklahoma, Norman, OK, USA. He has held various affiliated positions in the U.S. and Japan, including Adjunct Professor at the University of Illinois at Urbana-Champaign, Adjunct Professor at the University of Oklahoma, and Lecturer at UCLA, the University of Hawaii at Manoa, the University of Tokyo and the University of Cape Town. Prof. Kang received his PhD from UCLA, his MS from Michigan State University, and his BS from Seoul National University.*

Prof. Kang is a Fellow of Post-Tensioning Institute (PTI) and a Fellow of American Concrete Institute (ACI). Prof. Kang received the Kenneth B. Bondy Award for Most Meritorious Technical Paper as Lead Author from PTI in 2012, and the Wason Medal for Most Meritorious Paper as Lead Author from ACI in 2009. He regularly teaches the course of Post-Tensioned Concrete Structures at the University of Illinois at Urbana-Champaign every other summer (both on campus and online) and at the University of Hawaii at Manoa every fall and the University of Cape Town every other fall (real-time online lectures). Prof. Kang has served as an Editor-in-Chief for four journals: Wind and Structures, International Journal of Concrete Structures and Materials, Journal of Structural Integrity and Maintenance, and Advances in Computational Design; and as Associate Editor for PTI Journal of Post-Tensioning Institute. He is one of the founding and voting members of PTI DC-20 Committee, Building Design; and has been a voting member for a variety of technical committees, including: ACI Subcommittee 318-T, Structural Concrete Building Code – Post-Tensioned Concrete; ACI Committee 369, Seismic Repair and Rehabilitation; Joint ACI-PTI Committee 320, Post-Tensioned Concrete Building Code; Joint ACI-ASCE Committees 335, Composite and Hybrid Structures; 352 Joints and Connections in Monolithic Concrete Structures; and 423, Prestressed Concrete; and Joint ACI-ASME Committee 359, Concrete Containments for Nuclear Reactors.

Prof. Kang published more than 140 international journal papers (as of Jan. 2021), including over 45 in ACI Structural Journal and over 10 in PTI Journal, and more than 100 international conference proceedings. He has chaired numerous sessions/symposiums of structural engineering; delivered many plenary/keynote/invited speeches; and organized several international conferences/workshops as a Chair.

Additionally, Dr. Kang has done a lot of practices as a consulting engineer in Korea and the U.S. Prior to joining the academia, he had a working experience in California, USA (e.g., John A. Martin & Associates), and was a licensed Professor Engineer (PE) in California. He is currently working on the smart stressing system as a Consultant with EVEHX, a world-leading company in the area of post-tensioning headquartered in Brazil. Prof. Kang has also been working on the adoption of newer technologies such as artificial intelligence (AI) for the performance-based design in wind engineering, and holds over 20 registered patents in the U.S., Korea, Canada, China, EU (France, U.K., Italy, Spain, Switzerland, Germany), Thailand, and Australia.

Abstracts of Selected Recent Papers and Patent

Impact Behavior of Unbonded Post-Tensioned Concrete Beams (by A. Nghiem, C. Demartino, Y. Xiao, and T. H.-K. Kang; ACI Structural Journal, V. 118, No. 1, Jan.-Feb. 2021)

This study experimentally investigates the effects of the unbonded post-tensioning on the response of reinforced concrete (RC) beams under impact loads. A total of fifteen specimens were cast and tested. All specimens had identical longitudinal reinforcement, but varying shear reinforcement ratios designed to be both flexural and shear-deficient in static conditions according to the ACI code. In particular, thirteen unbonded post-tensioned (PT) beams were tested under drop-weight impact applied at the midspan in simply supported conditions and compared with conventional type RC beams. The main variables investigated include increasing levels of PT force and the application of two different impact energies per each specimen type, shear- or flexural-deficient. The experimental results showed that the levels of PT force and shear reinforcements of the specimens played an important role in their overall behavior. With respect to beneficial design recommendations, relationships between the impact resistance and the static capacity are provided; a general increase in strength of around three times that of the static capacity is observed when impacted. Additionally, relationships between the ratio of the impact energy to static capacity are developed with regard to the maximum and residual member displacements.

Performance-Based Design of Tall Buildings for Wind Load and Application of Response Modification Factor (by H. Alinejad, S. Y. Jeong, and T. H.-K. Kang; Wind and Structures, V. 31, No. 2, Aug. 2020)

In the design of buildings, lateral loading is one of the most important factors considered by structural designers. The concept of performance-based design (PBD) is well developed for seismic load. Whereas, wind design is mainly based on elastic analysis for both serviceability and strength. For tall buildings subject to extreme wind load, inelastic behavior and application of the concept of PBD bear consideration. For seismic design, current practice primarily presumes inelastic behavior of the structure and that energy is dissipated by plastic deformation. However, due to analysis complexity and computational cost, calculations used to predict inelastic behavior are often performed using elastic analysis and a response modification factor (R). Inelastic analysis is optionally performed to check the accuracy of the design. In this paper, a framework for application of an R factor for wind design is proposed. Theoretical background on the application and implementation is provided. Moreover, seismic and wind fatigue issues are explained for the purpose of quantifying the modification factor R for wind design.

Seismic Performance of Moderately Short Concrete Coupling Beams with Various Reinforcements (by W. S. Park, T. H.-K. Kang, S. Kim, and H.-D. Yun; ACI Structural Journal, V. 117, No. 3, May-June 2020)

The purpose of this study is to investigate the effect of various reinforcement configurations on the seismic performance of diagonally reinforced coupling beams in part of coupled reinforced concrete wall systems. A total of four approximately half-scale concrete coupling beams were fabricated between concrete blocks and tested under cyclic shear distortions in a double curvature condition. All four specimens had the same clear span-depth ratio (l_n/h) of 2 and the same reinforcement except for the transverse reinforcing details and presence of steel fibers. The control reinforced concrete (RC) coupling beam was designed with full section confinement according to the seismic provisions of the ACI 318-19 code, except for the steel volume, whereas the other specimens were provided with reduced transverse reinforcement and/or steel fibers for the purpose of improving the constructability. The top and bottom horizontal bars were sufficiently embedded into the wall as opposed to the ACI 318-19 recommendation. Test results indicate that the transverse reinforcement configuration and horizontal reinforcement embedment had a significant impact on the behavior both at the linear and nonlinear deformation ranges. For the coupling beams confined only by closed outer stirrups but without inner crossties, the addition of hooked steel fibers at a volume fraction of 0.75% provided similar structural performance compared with the RC coupling beam featuring full section confinement.

Grouted Extruded-Strand Tendons: Friction Coefficients and Differential Individual Strand Forces (by H. Shin, T. H.-K. Kang, and J.-H. Park; ACI Structural Journal, V. 117, No. 3, May-June 2020)

Due to increasing demand and application of grouted extruded- strand tendons, need for analysis of tendon characteristics for design and construction exists. Measured for this paper were friction coefficients and strand tensile force distribution of horizontal circumferential tendons of a nuclear containment structure. Results indicated that grouted extruded-strand tendons had very low curvature and wobble friction coefficients (μ = 0.0277/rad and k = 0.0006/m [0.00018/ft]) in comparison to that observed for grease-filled bare-strand tendons. Furthermore, individual strand tensile forces in grouted extruded-strand tendons achieved lower standard deviation than that of bare-strand tendons.

Bridging Nodal Aberration Theory to designing Optical Systems with Freeform Optics

by Jannick P. Rolland, Member EUAS

Short Biography
Prof. of Optics, The Institute of Optics, University of Rochester NY
Endowed in 2009 as the Brian J. Thompson Professor of Optical Engineering
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Director of the R.E. Hopkins Center 2012-present
2013-present CEO/CTO and Board Member of LighTopTech Corp.
1996-2006 On Editorial Board of the Journal Presence (MIT Press)
1999-2004 Associate Editor of Optical Engineering
2016-2022 Topical Editor of Optics Letters, an OSA Journal
Fellow of the National Academic of Inventors (NAI), OSA, SPIE, and NYSTAR
2014 Recipient of the David Richardson Medal
2107 Edmund A. Hajim Outstanding Faculty Award
2018 Recognized by AWE as one of 8 influential women pioneer in Augmented and Virtual Reality
2019 Alumna of the Year in Optical Sciences at the University of Arizona
2020 Recipient of the Joseph Fraunhofer Award / Robert M. Burley Prize
55 patents and over 500 publications

Freeform optics is self-assured to revolutionize the optical systems of our collective future, including high precision imaging systems. Nodal Aberration Theory (NAT) invented in the 1980s was conceived initially to understand the aberrations of misaligned optical systems. Around 2010 it was realized that NAT can serve as the foundation for expressing the optical aberrations of freeform optics systems. The impact of moving from 100 years of design with rotationally symmetric surfaces (or sections of) into freeform optics is tremendous and opens the design space towards higher performance, more aggressive specifications in the field of view and F/#, more compact solutions, broadband solutions, and distortion-free or distortion-tailored designs.

1. Nodal Aberration Theory

In 1976 on top of Kitt Peak in Arizona, astronomers acquired a through-focus star plate shown in Fig. 1 with a 90-inch Ritchey-Chrétien telescope. The star plate, shown in Fig. 1, was first reported in a 2005 publication by Kevin P. Thompson and was adapted here to indicate two nodes of zero astigmatism within the full field of view (FOV) [1]. Beware of how the nodes display in the field, either symmetrically around the field center or with an offset denoted in the picture as $\mathbf{a}_{222}$. Bold in this paper denotes vectors. The dark blue hyperbolas on the star plate indicate the orientation of the sagittal lines sampled throughout the FOV.

Shack and Thompson developed the mathematics of Nodal Aberration Theory (NAT) [2]. They showed that the wave aberration function *W* could be expanded as a scalar function of two vectors, the normalized pupil vector $\boldsymbol{\rho}$ and the normalized field $\boldsymbol{H}$. The system aberrations are then obtained by summing over the surface contributions. They also established that in the case of a Ritchey-Chrétien telescope, such as the Hubble telescope, a common state of misalignment led to *binodal astigmatism* (i.e, meaning two nodes or zero of astigmatism), but interestingly with one node near the center of the field, which was not what was observed in the star plate. Tobias Schmid *et al.* further validated this finding [3, 4]. Thus, the pattern of astigmatism seen in Fig.1 cannot be explained with sole misalignment. Thompson went on in his Ph.D. thesis to mention another critical factor in large telescopes that he called "mirror warpage" that may result from an improperly supported primary. Thompson recognized then that warpage would introduce field-constant astigmatism that will contribute to the vector $\mathbf{b}_{222}$ shown in Fig. 1 as $\mathbf{f}_{222}$. Schmid *et al*., in 2008, studied adding an astigmatic figure error located in the aperture stop of a Ritchey-Chrétien telescope to aim at understanding and quantifying the locations of the nodes in binodal astigmatism induced by figure error or misalignment or in combination [5]. This investigation closed the loop on understanding the 1976 star-plate acquired on Kitt Peak, which was caused by a combination of misalignment and figure error.

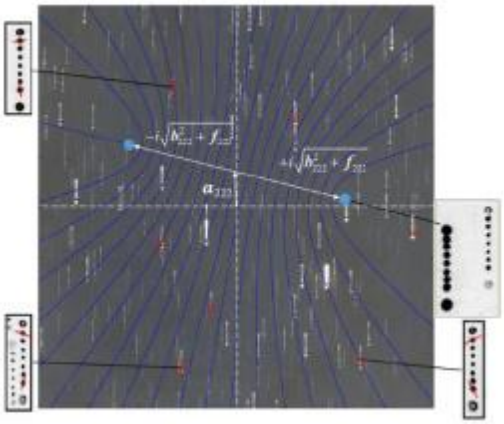

Figure 3. Through-focus photographic star plate, taken with the 90-in telescope of the Steward Observatory, located on Kitt Peak. The boxes to the left and right of the plate are magnified regions of the star plate showing no astigmatism at two nodes (one node is shown) in the full FOV of the telescope (Adapted from Fig. (1)[1]).

2. Mount-Error as a Step to Revealing FReeform Aberrations

Nodal Aberration Theory, which only accounted for rotationally symmetric surfaces, included the development of NAT up to 5th order aberrations that revealed to be important in the expansion of NAT to account for freeform surfaces [1, 6-8]. In 2012, Fuerschbach *et al.* extended the concept of figure error into freeform surfaces [9]. What led to this major step was the realization that different types of mounting points on a mirror could be modeled with Zernike polynomials and used to predict various surface deformations when influenced by gravity. The mathematical analysis detailed in [9] reveals that the use of a conjugate vector first introduced in NAT enables explaining field-conjugate field-linear astigmatism, whose field dependency is illustrated in Fig. 2b. Accurately, the equation found in Fuerschbach *et al.* to describe field-conjugate field-linear astigmatism was a

component in the expression of field-quartic fifth order astigmatism of NAT (i.e. Eq. (23) in [8]). It was also first found as a limiting aberration in Stacy and Macenka (i.e., Fig. 7 of [10]) who recognized the field-linear dependence of astigmatism, but the analytic origin remained unknown. A significant finding of Fuerschbach *et al.* was that the aberrations induced by freeform surfaces were linked to 5th order aberrations in NAT.

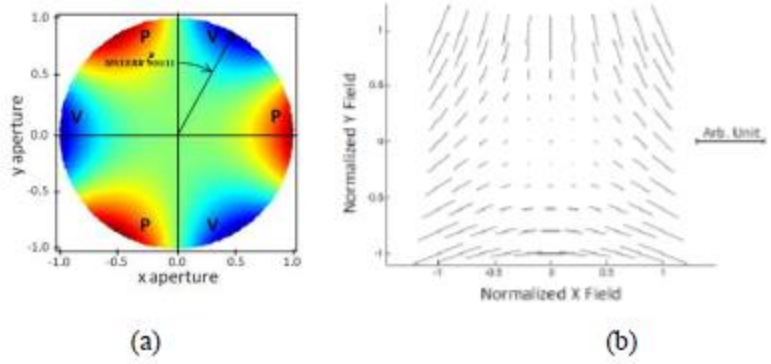

Figure 2. Concept of field-conjugate field-linear astigmatism induced by a kinematic three-point mount: (a) Topographic map describing trefoil as a figure error on a surface away from the stop in arbitrary units; *P* and *V* denote Peak and Valley points in the topographic map where the magnitude and orientation of the deformation are given respectively by $_{\text{MNTERR}}|z_{10/11}|$ and $_{\text{MNTERR}}\xi_{10/11}$ with the clocking angle defined to the y-axis, z10/11 are the coefficients of Zernike trefoil Z10/11 used to characterize the mount error (i.e., MNTERR); (b) Illustration of the field dependence of field-conjugate field-linear astigmatism generated by a mount-induced trefoil deformation clocked at zero degrees angle (Adapted from [9]).

3. Aberration Theory of Freeform Surfaces

Building on the findings of adding a trefoil deformation away from the aperture stop in an optical system, any freeform surface in an optical system or deformations induced by a mounting geometry will create a field constant of that aberration. It will also develop aberrations of lower radial order of the aperture dependence with a field dependency we may find described in the aberration theory NAT of tilted and decentered systems [1, 6-8]. To isolate the contribution of each freeform shape to the aberration fields, Fuerschbach continued to work with a Schmidt telescope with a sufficiently small enough FOV not to be limited by higher-order aberrations. Fuerschbach went on to establish the field dependence and nodal behavior of each FRINGE Zernike freeform surface. This knowledge turns out to be critical to the design of freeform optical systems [11].

4. Freeform Aberration Theory

In 2018, Aaron Bauer et al. developed a novel design method using the freeform aberrations [12]. Bauer et al. found a means of selecting the best folding geometry in a three-mirror unobscured freeform imager, and ranking others. Folding geometries of a three-mirror imager were investigated, shown in Fig. 4, where the winner is Tier 1, and Tier 4 are the least favorable geometries.

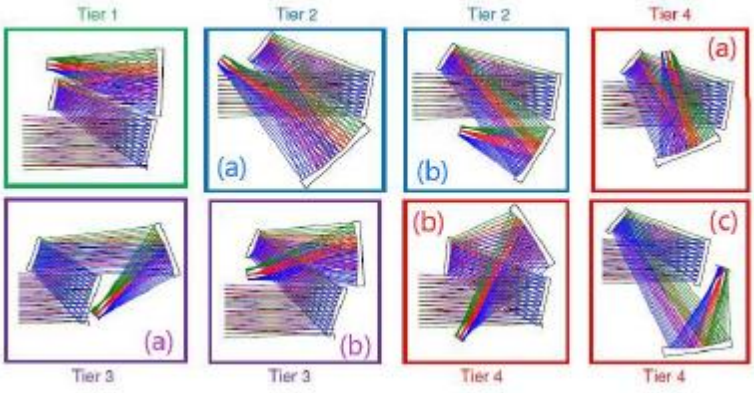

Figure 4. Ranking of various folding geometries by Tier, where Tier 1 is the winner take all for this power distribution of the mirrors (Adapted from [12])

Bauer *et al.* went on to develop and demonstrate a step-by-step method of optimizing freeform optical systems based on the visualization of various aberrations using full field displays. While designing with a set of specifications, the designer must maintain the overall freeform sag departures to a minimum to improve manufacturability, where the speed of fabrication and testability are both of consideration [13, 14]. To further ensure this minimum and further help the design process, metrics to constrain either the RMS sag departure or the RMS gradient normal departure, depending on the type of orthogonal polynomials used, were then reported [15, 16]. Also, in the methodology of Bauer *et al.*, it is worth noting that the starting points satisfy first-order specifications but are not corrected for 3rd order aberrations as done in our earlier approach to design before the theory of freeform aberrations and the Bauer method were developed [17]. Also, significant field-asymmetric field-linear astigmatism and field-conjugate field-linear astigmatism are often present. They reveal why freeform surfaces are useful in improving the performance of asymmetric optical systems. Also worth noting is the awareness of various types of degeneracies in design that, if mitigated, as done as part of our design methods, ensure optimal outcomes in optimization [18].

Dramatic advances in both optical performance and system packaging of imaging systems are enabled by freeform optical components. Examples of designs performed in our group to date include dispersive spectrometers [19, 20], viewfinders [21, 22], and three-mirror imagers [23, 24]. The field of freeform optical design is growing in the community and a review paper on freeform optics includes a comprehensive list of work by others as well [25].

Acknowledgements

This work synergizes with the National Science Foundation I/UCRC Center for Freeform Optics (IIP-1338877, IIP-1338898, IIP-1822026, IIP-1822049) and its industry and government members (https://centerfreeformoptics.org).

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Drop Self-Shaping & Self-Bursting: New Approaches to obtain Regularly Shaped Micro- & Nanoparticles

by Nikolai Denkov, Member EUAS

Short Biography

Professor DSc Nikolai Denkov (MAE) is Head of the Laboratory "Active formulations and materials" at the Department of Chemical & Pharmaceutical Engineering in Sofia University, Bulgaria. His research includes experimental and theoretical studies on the formation, stability, rheology and applications of various disperse systems, and on the surfactant control of their properties. He has published > 175 research articles, including 2 papers in Nature, 1 in Nature Commun. and 17 invited reviews, cited > 8500 times in literature (h-index = 45). He was visiting researcher in JRDC (Japan), senior researcher in Rhone-Poulenc R&D (France), lead scientist in Unilever R&D (USA) and guest professor in France (ESPCI-Paris and Univ. Lille). For his achievements, in 2019 Prof. Denkov was awarded the Solvay Prize of the European Colloid and Interface Society (ECIS) and was elected as a regular member of Academia Europaea. In 2020 he received the Lectureship Award of the Division of Colloid and Surface Chemistry in Japan. He is recipient of the highest national award for scientific achievements "Pythagoras" by the Bulgarian ministry of education and science (2010).

The search for active micro- and nano-particles[1-3] exploded in the last years due to the rapid advance in several related research areas – origin of life[4,5], artificial life[6], soft robotics and nanomedicine[7]. Although each of these areas has its own approach and specific aims, all they share the needs to understand (1) how the nature achieves the highly synchronized dynamic organization of so complex structures with multiple functionalities, (2) how these structures emerged and evolved on Earth, and (3) how we could replicate and advance them in a way which is useful to the humankind. Therefore, numerous approaches were proposed for fabrication of active particles of millimeter or micrometer size.[1-7] Most of the active particles proposed in the literature are activated by external forces, e.g. electric, magnetic or electro-magnetic fields, including light, or by release of pre-loaded "fuel" molecules.

Recently, we discovered a conceptually new type of self-assembling micro-particles[8-9]. These particles exhibit several types of complex activities which are typical for the living organisms, while being composed of very simple chemical components only: non-polar oily phase (*e.g.* alkanes, fatty alcohols, triacylglycerols or their mixtures), dispersed as micrometer sized drops in an aqueous phase containing long-chain surfactant molecules which form adsorption layer on the drop surface and stabilize the droplets against

coalescence. Some of the "activities" performed by these oily droplets are illustrated in Figure 1 and include:

(a) Spontaneous **drop self-shaping** into different fluid polyhedra; hexagonal, tetragonal and triangular platelets; and long thin rods and fibers (Figure 1a-d). All of these shapes can be formed "on demand" using appropriate control of the experimental conditions.[8,9] Furthermore, polymeric particles with the respective shapes were also prepared which have potential applications in several areas.[10]

(b) Spontaneous **particle self-bursting** upon cooling and/or heating, with formation of nano-particles, without any mechanical energy input to the system (Figure 1f-j). Nano-drops and nanoparticles with size of *ca.* 20-50 nm for emulsified triacylglycerols and ca. 200-500 nm for alkanes were obtained.[11-13] The obtained lipid nanoparticles are of great interest as potential drug carriers in medical and pharmaceutical applications.

(c) Formation of **flagellated swimmers** without using external forces or triggers (Figure 1e).

(d) **Engulfment** of the surrounding medium in the form of aqueous micro- and nano-droplets.[13]

All these activities occur spontaneously when oily emulsion drops are dispersed in aqueous surfactant solution and the temperature of the environment is varied in a relatively narrow range of *ca.* ± 5°C around the melting temperature of the oily phase, similar to the temperature variations in the natural water pools during the day-night cycle. No external forces, gradients of external fields, or gradients of dissolved substances are needed to trigger them. For control of these activities, one can use different cooling/heating protocols, oils with appropriate melting temperature, or surfactants with specific head-groups and chain-lengths.[8-13]

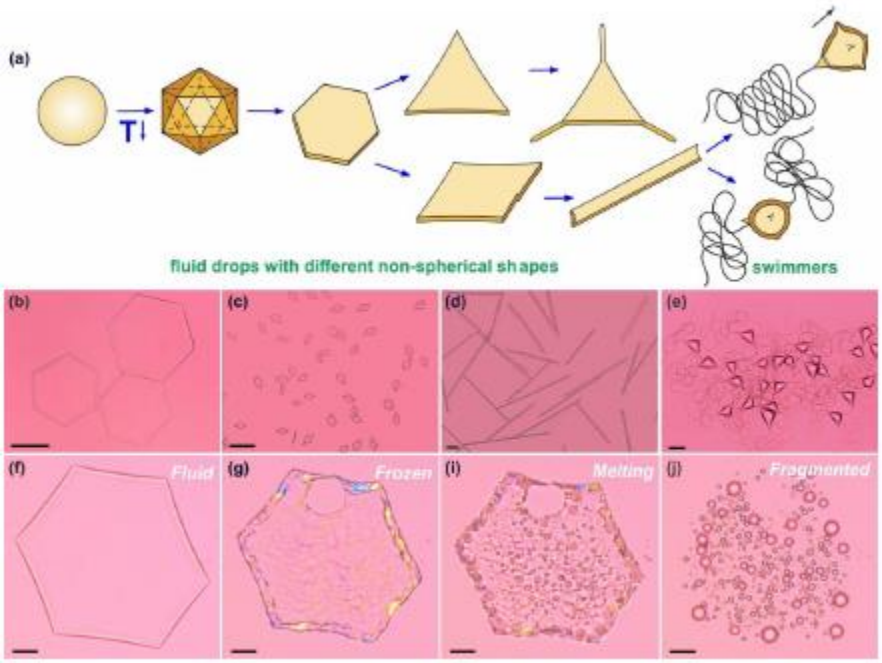

Fig. 1 (a) Drop shape evolutionary scheme observed upon cooling of emulsion drops of hydrophobic phase (oil) dispersed in aqueous solution of a long-chain surfactant. The drops have characteristic spherical shape at high temperatures. Upon cooling, they transform into regular polyhedra which gradually flatten into hexagonal fluid platelets. Afterwards, triangular or tetragonal platelets form which further evolve into long rod-like particles which may turn into drop extruding thin fibers, thus forming micro-swimmers. (b-f) Fluid

non-spherical drops with various shapes: (b,f) hexagonal platelets; (c) tetragonal platelets; (d) rod-like particles; (e) bacteria-shaped drops with flagella which swim with a velocity of *ca.* 0.5 μm/s. Besides self-shaping and swimming, these drops are able to spontaneously divide and burst as well. The bursting process is very efficient, especially when observed upon heating, as shown in (g-j) - the frozen platelet formed from a single oil drop (g) melts into hundreds of separate drops (i-j). These figures are adapted from Refs. [9,11]. The horizontal dark bars correspond to 20 μm.

The simplicity of the system and the various possible behaviors cause these microparticles to attract the interest for modelling and studying the processes of morphogenesis in living and non-living matter, micro-swimming, division and endocytosis in non-living systems, which is of great interest in the areas of origin of life, artificial life and soft micro/nano-robotics.

The mechanism explaining the observed deformations is schematically presented in Figure 2 and can be briefly explained as follows: upon cooling, the surfactant adsorption layer freezes first and then serves as a 2D template for inner ordering of the oily molecules next to the drop surface. These molecules arrange in thin layers (ca. 10 to 100 nm thickness) of the so-called rotator phase.[14] Molecules arranged in rotator phases possess a long-range positional order while preserving certain mobility to rotate, which results in a complex visco-plastic rheological behavior.[15] Therefore the rotator phases have sufficiently high mechanical strength to counteract the capillary pressure at the oil-water interface which tries to minimize the oil-water interfacial area (causing the spherical shape of small droplets). The layers of rotator phase are dynamic (it is a fluid phase) and the subtle interplay between the rotator phase nucleation and growth, on one hand, and the capillary phenomena, on the other hand, lead to the formation of the dynamic complex drop shapes observed experimentally.[14-17] The observed self-shaping sequence was successfully described by a theoretical model which considered the energy balance between the positive drop surface energy and the negative energy of rotator phase formation, with the assumption that the rotator phase forms at the edges of the deforming particle only.[18,19]

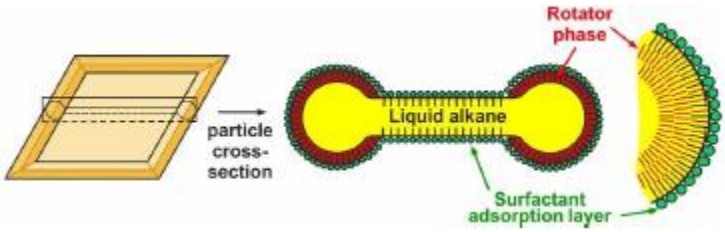

Fig. 2 Role of surface freezing and rotator phases for the formation of shaped drops in cooled emulsions. Note that thin layers of rotator phase are formed only in the curved regions at the drop periphery.[9]

The shapes observed with the oily drops resemble closely the shapes of many diatoms - major group of microalgae, found in the waterways, oceans and soils around the world. Based on this shape similarity, Gordon et al.[20] hypothesized that such polygonal shapes may emerge in nature as a result of force and momentum balances, typical for the so-called "tensegrity" structures which has been introduced as a concept by Buckminster Fuller in 1960s and is currently used in various engineering constructions. In our case, this "tensegrity" structure is formed by the frame of plastic rotator phase, formed at the drop periphery, and the oil-water interfacial tension which compresses the plastic structure and

maintains its balanse.[18-20]

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Enhancing DLV for Large-Scale Reasoning

by Nicola Leone, Member EUAS

Short Biography

Nicola Leone is the Rector of University of Calabria. He is professor of Computer Science, and he previously was professor of Database Systems at Vienna University of Technology until 2000. At the University of Calabria, he has served as the Chair of the Degree Program of Computer Science 2001-2008, and as the head of the department of Mathematics and Computer Science 2008-2018. He has been elected as the Rector of University of Calabria 2019-2026.

He is internationally renowned for his research on Knowledge Representation, Answer Set Programming (ASP), and Database Theory, and for the development of DLV, a state-of-the-art ASP system which is popular world-wide.

He published more than 250 papers in prestigious conferences and journals, and 12,000 citations, with h-index 56.

He is area editor of the TPLP journal (Cambridge Press) for "Knowledge Representation and Nonmonotonic Reasoning", and been Keynote Speaker and Program Chair of several international conferences, including, e.g., ICLP, JELIA and LPNMR.

He is recipient of two Test-of-Time awards from the ACM and ALP, and winner of many Best Paper Awards in top-level AI conferences.

He is a fellow of EurAI, Honorary professor at TUWIen, and member of EU Academy of Sciences.

Enhancing DLV for Large-Scale Reasoning

Abstract

DLV is an advanced logic-based system for knowledge representation and reasoning, which has been successfully employed in academy and industry for the development of AI applications.

Several real-world applications of DLV made evident the need for efficiently handling multiple queries and reasoning tasks over large-sized knowledge bases. In this paper we present some recent enhancements in the ASP system DLV2 for enabling reasoning over large-scale domains. In particular, we developed both an optimized implementation, sensibly reducing memory consumption, and a server-like behavior to support efficiently multiple-query scenarios. The high potential of DLV2 for large-scale reasoning is outlined by the results of an experiment on data-intensive benchmarks. The applicability of the system in real-world scenarios is demonstrated employing DLV2 as reasoning service to query, in natural language, the large DBpedia knowledge base. The relevance and the high potential industrial value of this research is also confirmed by the direct interest of a major international industrial player, which has stimulated and partially supported this work.

Enhancing Magic Sets with an Application to Ontological Reasoning

Published online by Cambridge University Press: **20 September 2019**

Abstract

AI systems perform very complex tasks and need advanced optimization methods to achieve good performance.
Magic sets are a Datalog to Datalog rewriting technique to optimize query answering in logic-based systems. The rewritten program focuses on a portion of the stable model(s) of the input program which is sufficient to answer the given query. However, the rewriting may introduce new recursive definitions, which can involve even negation and aggregations, and may slow down program evaluation. This paper enhances the magic set technique by preventing the creation of (new) recursive definitions in the rewritten program. It turns out that the new version of magic sets is closed for Datalog programs with stratified negation and aggregations, which is very convenient to obtain efficient computation of the stable model of the rewritten program. Moreover, the rewritten program is further optimized by the elimination of subsumed rules and by the efficient handling of the cases where binding propagation is lost. The research was stimulated by a challenge on the exploitation of Datalog/DLV for efficient reasoning on large ontologies. All proposed techniques have been hence implemented in the DLV system, and tested for ontological reasoning, confirming their effectiveness.

Fast Query Answering over Existential Rules

Publication:ACM Transactions on Computational Logic
March 2019 Article No.: 12 https://doi.org/10.1145/3308448

Abstract

Enhancing Datalog with existential quantification gives rise to Datalog$^{\exists}$, a powerful knowledge representation language widely used in ontology-based query answering. In this setting, a conjunctive query is evaluated over a Datalog$^{\exists}$ program consisting of extensional data paired with so-called “existential” rules. Owing to their high expressiveness, such rules make the evaluation of queries undecidable, even when the latter are atomic. Decidable generalizations of Datalog by existential rules have been proposed in the literature (such as weakly acyclic and weakly guarded); but they pay the price of higher computational complexity, hindering the implementation of effective systems. Conversely, the results in this article demonstrate that it is definitely possible to enable fast yet powerful query answering over existential rules that strictly generalize Datalog by ensuring decidability without any complexity overhead. On the theoretical side, we define the class of parsimonious programs that guarantees decidability of atomic queries. We then

strengthen this class to strongly parsimonious programs ensuring decidability also for conjunctive queries. Since parsimony is an undecidable property, we single out Shy, an easily recognizable class of strongly parsimonious programs that generalizes Datalog while preserving its complexity even under conjunctive queries. Shy also generalizes the class of linear existential programs, while it is uncomparable to the other main classes ensuring decidability. On the practical side, we exploit our results to implement DLV$^{\exists}$, an effective system for query answering over parsimonious existential rules. To assess its efficiency, we carry out an experimental analysis, evaluating DLV$^{\exists}$ performances for ontology-based query answering on both real-world and synthetic ontologies.

Tailoring Structure and Properties in Metastable Materials

by Jürgen Eckert, Member EUAS

Short Biography

Jürgen Eckert obtained his Ph.D. (German: Dr.-Ing.) in Materials Science and Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany in 1990. Already at that time his research focused on the synthesis and property characterization of metastable materials, including amorphous, quasicrystalline and nanocrystalline alloys and composites. After his Ph.D. he worked for two and a half years as postdoc at the California Institute of Technology. After a short break in industry, he moved to the Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, one of the leading Materials Research Science Centers in Germany. From 1996 until 2003 he acted as Head of the Department Metastable and Nanostructured Materials at IFW Dresden, before moving to TU Darmstadt as Full Professor for Physical Metallurgy. In 2006 he moved back to Dresden as Director of the Institute for Complex Materials at IFW Dresden and Chair for Synthesis and Analysis of Materials at Dresden University of Technology (TU) Dresden. In 2013/2014 he served as the Scientific Director of IFW Dresden. In 2015 he moved to Austria as Chair Professor of Materials Physics at Montanuniversität Leoben, and Director of the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences. He also held an Adjunct Professor Position at Michigan Technological University, Houghton, USA between 2002 and 2005, and was a Visiting Professor at University of Vienna, Austria at the Institute of Physics, Physics of Nanostructured Materials (2009 / 2010 / 2012).

He is an international expert in the field of metastable materials and has published more than 1200 papers in archival journals (h-index: 88 (WoSci), more than 37.000 citations). He also published more than 150 conference papers, 18 book chapters, edited 6 books, conference proceedings and journal issues, holds more than 20 patents, and delivered so far more than 220 plenary, keynote and invited presentations.

Jürgen Eckert was honored as Dr. honoris causa (Dr. h.c.) by the Slovak University of Technology in Bratislava, Slovak Republic (2012), and received the Gottfried Wilhelm Leibniz Award of the German Research Foundation (2009), the highest Science Prize and scientific honor in Germany. Other honors include the DGM-Prize 2014 of the German Materials Research Society, an ERC Advanced Grant of the European Research Council (2013), the ISMANAM Senior Scientist Award (2012), the Hsun Lee Lecture Award of the Chinese Academy of Sciences (2006), the Georg-Sachs-Prize of the German Materials Research Society and the Austrian Metal Industry (1997), and the FEMS Materials Science and Technology Prize of the Federation of European Materials Science Societies (FEMS) in 1997. He received the Young Scientist Award of the German Materials Research Society (1994), and the ISMANAM Young Scientist Award (1997). He is a corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences (2017), a Member of the European Academy of Sciences (2018) and has been elected to the class of 2018 MRS Fellows of the Materials Research Society, USA (2018). He was awarded an ERC-Proof of Concept Grant of the European Research Council (2019) for his work on thin film metallic glasses, and was elected as Honorary Member of The Indian Institute of Metals and as corresponding Member of the Section Technical Sciences of the Saxon Academy of Sciences and Humanities in Leipzig, Germany (2020).

Jürgen Eckert's scientific interests and research activities include phase formation, processing and structure-property correlations of metastable materials processed under non-equilibrium conditions; structural and functional materials and

metal matrix composites with particular emphasis on solidification fundamentals and solid state reactions; rapid solidification processing; additive manufacturing techniques; biocompatible, magnetic and superconducting materials, and materials for energy applications and energy harvesting (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen production and storage) and thin film systems for flexible electronics; solidification of metal matrix composites; mechanical and electrochemical properties of bulk materials, coatings and surfaces; biologically inspired far-from-equilibrium materials and architected structures; mathematical modelling of advanced materials and processes.

Over the years, Jürgen Eckert and his team have provided sustained contributions to research on metastable advanced high performance materials. Whereas early work focused on amorphization and quasicrystal formation in metallic systems, and fundamental observations on the development of nanoscale grain sizes in metallic materials, the interest shifted later on to the development and property optimization of bulk metallic glasses and composites, high entropy alloys and structurally modulated systems with hierarchically tuned microstructure. Significant attempts concentrated on developing plastically deformable and tough bulk metallic glasses and composites through a synergistic approach by understanding how atomic scale structures, microstructural features and stress, plus processing-induced heterogeneities determine the mechanisms of plastic deformation on different length scales such as to overcome the otherwise unavoidable brittleness of glassy materials. These activities developed into a general approach using disorder and heterogeneity concepts for creating new strategies for the design of advanced materials processed under highly non-equilibrium conditions. This concept allowed to create new high-strength lightweight alloys, hard and soft magnetic materials, porous bulk materials and hybrid structures for biomedical applications, materials for energy applications (metals, oxides, hierarchical carbon structures), and also touched on surface modification and development of architected gradient structures.

Jürgen Eckert's recent research activities focus on the development and application of methods for in-depth *in situ* and in operando investigation of phase transformations and structure-property correlations using local probes and high resolution techniques for structure characterization and imaging of local structures, chemical compositions and interaction of nanoscale objects with external fields and stimuli (e.g. mechanical, thermal, electrical, magnetic fields). This allows creating tailored biologically inspired far-from-equilibrium materials with hierarchical structure and tuned disorder *in situ*. This can be realized in a microscope or through flash annealing at extreme heating and cooling rates. An example for such materials is the *in situ* design and testing of glassy metallic structures containing heterogeneities on different length-scales to overcome their intrinsic brittleness. These heterogeneities can be induced through local chemical variations, variations in short- or medium-ranger order or through introducing locally varying stress/strain states. The concept of *in situ* design and testing is applicable to bulk structures and thin film systems and to a wide range of materials, and is therefore expected to open

a new research avenue for creating materials with unique properties by design. Some of the key publications in this area include:

- I. Okulov, I. Soldatov, I. Kaban, B. Sarac, F. Spieckermann, J. Eckert, "Fabrication of Metastable Crystalline Composites by Flash Annealing of $Cu_{47.5}Zr_{47.5}Al_5$ Metallic Glass Using Joule Heating", *Nanomaterials* **10**, 84 (2020).
- D. Şopu, S. Scudino, X.L. Bian, C. Gammer, J. Eckert, "Atomic-Scale Origin of Shear Band Multiplication in Heterogeneous Metallic Glasses", *Scripta Mater.* **178**, 57 (2020).
- L. Zhang, R.L. Narayan, B.A. Sun, T.Y. Yan, U. Ramamurty, J. Eckert, H.F. Zhang, "Cooperative Shear in Bulk Metallic Glass Composites Containing Metastable β-Ti Dendrites", *Phys. Rev. Lett.* **125**, 055501 (2020).
- C. X.L. Bian, D. Şopu, G. Wang, B.A. Sun, J. Bednarčik, C. Gammer, Q.J. Zhai, J. Eckert, "Signature of Local Stress States in the Deformation Behavior of Metallic Glasses", *NPG Asia Mater.* **12**, 59 (2020).
- B. Sarac, T. Karazehir, Yu.P. Ivanov, B. Putz, A.L. Greer, A.S. Sarac, J. Eckert, "Effective Electrocatalytic Methanol Oxidation of Pd-Based Metallic Glass Nanofilms", *Nanoscale* **12**, 22586 (2020).

The long-term perspective of this research is to advance the understanding of structure-property correlations for hierarchically modulated structures and disordered systems over a variety of different length-scales under highly non-equilibrium thermodynamic and kinetic conditions. This shall evolve into a comprehensive description of phase formation, transformation, dynamics and property design under extreme conditions, such as ultra-fast heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimuli. Whereas some of these approaches are already followed for crystalline materials, research on disordered and interface dominated heterogeneous materials along these lines touches almost unknown grounds, since the structural diversity introduced through disorder and local distortion opens up new avenues for overcoming the compositional and structural constraints of crystalline materials.

The ability to predict and design disorder in architected materials with unique functionality provides vast opportunities for new property-optimized materials including high-strength-lightweight systems, biomedical implants, micromechanical components or modulated thin film systems for energy storage and harvesting with unique performance characteristics. Along this line not only the basic fundamental mechanisms of structure formation and property tuning are in the focus, but also the question how the findings can be transferred into parts, devices and systems for high performance structural and functional applications. For example, new flexible

microelectronic systems, novel materials and devices for energy storage and harvesting, or biocompatible (biodegradable) bulk materials, porous structures, coatings and surfaces can be realized, e.g. for tailored orthopedic implants, personalized medical devices, miniaturized hydrogen storage systems or functional membranes.

For creating such materials and structures, state-of-the-art techniques of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and also structure-biological mimetic and 3d printing techniques are used to generate hierarchically modulated heterogeneous materials. Multi-scale modelling techniques based on hierarchies of overlapping scales including quantum mechanics based structure modelling, atomistic modelling and numerical methods supplement the experiments. Machine learning algorithms for characterizing (local) property statistics not assessable with direct measurements can be employed for determining optimized materials with tailored properties or property combinations. This is vital for property-directed material design of disordered systems, and promises to open new routes for nanoscale structure formation in architected materials with unique functionality through generating an atomic structural – functional understanding of properties, performance and correlation of hierarchical thin film structures and membranes. Also tailored interface structures, nano- and multiscale hybrid systems and heterogeneous materials with locally modulated structure and properties can be generated through this approach.

Improvements in Cardiovascular Simulations, Coronary Stents & Cardiovascular Robotics

by Rafael Beyar, Member EUAS

Short Biography

Professor Rafael (Rafi) Beyar, is an interventional cardiologist, a biomedical engineer and an innovator, former director of Rambam Health Care Campus, Professor Emeritus of Medicine and Biomedical Engineering at the Technion and former Dean of the Faculty of Medicine. Beyar received an MD from Tel Aviv University, DSc in Biomedical Engineering from the Technion, and MPH from the Bloomberg School of Public Health, Johns Hopkins University. He trained at Rambam and Johns Hopkins Cardiology.

Beyar Research interests were cardiovascular simulations, coronary stents and cardiovascular robotics. He has authored more than 200 publications and 15 books, and is the recipient of numerous awards. He served as the Director of Interventional Cardiology at Rambam (1996–2006) and as Dean of the Rappaport Faculty of Medicine (1999–2004), establishing the Johns Hopkins Technion-Collaboration Program. During his term, Professors Hershko and Chiechanover were awarded the 2004 Nobel Prize in Chemistry. Beyar successfully led the hospital through the 2006 Second Lebanon War, when it was under missile attack. He led development of the hospital's 2,000-bed Fortified Underground Emergency Hospital, the Children's Hospital, the Oncology Center, and the Heart Hospital. Since 2018, the construction of the Health Discovery Tower, a premiere integrated research and innovation hub is underway, in collaboration with the academia and industry.

Beyar founded the hospital's technology transfer company, Rambam MedTech Ltd. (2014), and the MindUp Incubator on Digital Health with Rambam, Medtronic, IBM Pitango and Impact first in 2017. Beyar served as chair of the Israeli Basket Committee (2010–2014) and serves as the chair of the Steering Committee for the Israeli Organ Transplant Center since 2010.

Beyar co-founded InStent, which was acquired by Medtronic and NaviCath (later Corindus), a Technion Incubator Company, the first-in-the-world robotic coronary intervention, which was acquired by Siemens Healthineers (2019). He currently serves as director of BioRap of the Rappaport Institute and Rambam Med-Tech and is serving as director or advisor in several start-up companies. He founded and co-chairs with Professor Chaim Lotan the international meeting, Innovation in Cardiovascular Interventions (ICI) since 1996.

Perspective: Combining Medicine and Research, 5 Phases in my Career

The hypothesis behind my career is that combining medicine with engineering will create value for our patients and for the society. Continuing this thread from the

very beginning of my career, I never left this centerline in my various posts that I had to fill. I will describe below the evolving steps in the evolution of my career.

1. *Education*: Immediately after finishing my MD thesis I sought to get education in Biomedical Engineering. My research thesis was developing new methods for cardiopulmonary resuscitation (CPR) and cardiac assist by changing intrathoracic pressures.
2. *The Heart System Research Center at the Technion:* following my DSc thesis I was recruited as Faculty to the Department of Biomedical Engineer at the Technion. Together with Professor Sideman we founded the heart system research center which combines mechanics, circulation and metabolism with multimodality imaging and simulation. We established a word renown series of meetings and bool proceeding on complex modeling and analysis of the heart system.
3. *Internal Medicine and Cardiology training:* Not giving up of my clinical activity I completed my training in medicine and cardiology at Rambam Medicine and at Johns Hopkins Cardiology. I continued my cardiac-engineering projects in Johns Hopkins and based on our joint work the system for CPR was carried out in patients.
4. *Interventional Cardiology:* Following additional research and Clinical training in the University of Calgary, I founded the Unit of Interventional Cardiology at Rambam and served as head. I continued to advance novel engineering research applied to interventional cardiology as detailed below.
5. *Research and Development in Stents and Coronary Robotics;* I have founded InStent, one of the early bare metal stents company who developed self-expanding nitinol stents, as well as balloon expandable "BeStent" stents that reached global use in patients. Later, I founded Corindus as a Technion-Rambam endeavor which is now approved worldwide. Corindus is the first Robotic company for percutaneous coronary interventions. The CorPath GRX is now used in over 100 centers around the world.
6. *Dean of Medicine, Technion:* In the years 1999-2005 I was elected and served as Dean of the Faculty of Medicine at the Technion. Apart for expanding our educational programs introducing medicine-engineering tracks, I have established the Johns Hopkins – Technion collaboration program on Biomedical Science and engineering. In 2004, Professor Hershko and Ciechanover, faculty members in Medicine, with Professor Irvine Rose, got the Nobel award for the Ubiquitin protein degradation system.
7. *Director General Rambam Health Care Campus:* between 2006-2019, I was nominated and served as Director of the Rambam Health Care Campus. I built a new campus with the world renown fortified underground hospital for 2000 bed, now used for our COVID-19 patients, and above that a children hospital, a cancer center and a heart hospital. In the middle of the campus there is the Health Discovery Tower that will combine medicine, science and engineering, between the hospital and the surrounding academic and research

bodies. On top of that I established Rambam Med-Tech and the MindUP incubator on medical devices and digital health that is another important arms for continuing the vision of integrating medicine and engineering.

8. *Managing General Partner, Alive Israel Health Fund:* Continuing my clinical and research activities I co-founded Alive Health Venture Fund in 2020 in alliance with Maccabi Health Care and Assutah hospital. The fund invests in late stage medical device and digital health companies and provides a bridge for those successful companies to grow and achieve worldwide impact.

Numerical and Experimental Research on Risers and Pipelines

by Menglan Duan, Member EUAS

Short Biography

Prof. Dr. Menglan Duan held a Bachelor's degree (1987) in petroleum drilling engineering at the department of petroleum engineering, Jianghan University of Petroleum (Yangtze University since 2003), a Master's degree (1990) in offshore structural engineering and a Ph.D. degree (1993) respectively in petroleum mechanical engineering at the department of mechanical engineering, University of Petroleum of China. He served as senior engineer, research professor, chief engineer at the headquarter of China Classification Society from 1993 to 2006. In 2006, he joined the China University of Petroleum-Beijing as a professor of solid mechanics and ocean engineering, and is currently the Dean of Faculty of Safety and Ocean Engineering. He was Chairman of Specialist Committee V.8 Subsea Technology of the 20th International Ship and Offshore Structures Congress 2018, Chairman of China Branch of the Society for Underwater Technology, and a member of the EU Academy of Sciences.

Prof. Duan has published over 400 peer-reviewed journal papers, and coordinated over 180 projects in ocean engineering, mechanical engineering and petroleum engineering. His research covers a wide range of fields in marine risers, pipelines, subsea X-trees and connectors, square spudcan of Jack-up rig, anchor penetration, mooring system, integrity management of subsea production systems, cluster manifolds layout optimization, the ship attitudes; virtual Simulation, machinery intelligent diagnosis; adhesive Joints, welded structures, nanofibrous membranes; applied mathematical and mechanics et al. In the last seven years (2014-present), Prof. Duan has published 89 papers in prestigious international journals, with 37 of them summarized here and listed in references.

A large amount of theoretical, numerical and experimental works on risers and pipelines have been conducted by Prof. Duan in recent years. Deepwater steel lazy-wave riser [1-6] includes the large deformation behavior, under ocean current and internal flow, abandonment and recovery, transfer process during installation, under top end imposed excitations, and riser-soil interaction model effects. Theoretical models of viscoelastic damping of flexible risers and composite tensile armoured flexible pipes were developed [7-8]. The dynamic response of fluid-conveying pipes, curved pipes, inclined pipes, and dynamics and stability of pipe conveying two-phase flow [9] are further investigated. Vortex shedding characteristics, a VIV model for fatigue analysis of a marine drilling riser, and crack identification during deployment and retrieval were also analyzed. Severe Slugging and the interaction between severe slug buildup and dynamic response of a submerged top-tensioned riser were followed investigated. Other riser aspects on free-standing hybrid riser, reliability analysis and J-lay method of riser were explored.

Pipelines focused on the lateral and upheaval buckling of pipelines and pipe-in-pipe pipelines, indentation of Pipe-in-pipe Structures, collapse of sandwich pipes and thick-walled pipes, theoretical elastic and non-elastic buckling of pipes under external/internal pressure, mechanical behavior of ring-stiffened composite offshore rubber hose, thermal

behavior of multilayer pipeline with phase change material, and coiled tubing. Mode localization in lateral buckling of partially embedded submarine pipelines, prediction of the upheaval buckling critical force for imperfect submarine pipeline, lateral buckling critical force and a unified formula for the critical force for submarine pipe-in-pipe pipelines are presented [10-14]. Collapse of sandwich pipes with PVA fiber reinforced cementitious composites core, prediction of the collapse pressure for thick-walled pipes, on the external pressure capacity of deepwater sandwich pipes with inter-layer adhesion conditions, elastic and non-elastic buckling of pipes under external/internal pressures were parallelly investigated [15-19].

Transient thermal analyses of multilayer pipeline with MicroPCM particles [20-22] were carried out recently. A mathematical model was presented for the start-up and cool-down processes in a multilayer pipeline with an inner steel pipe, an intermediate PCM layer, and an external thermal insulation layer. With enthalpy formulation adopted for the PCM layer, the governing equations for heat conduction in the composite pipe walls and for energy transport in the produced fluid are solved numerically by explicit finite difference methods. The effects of the PCM thickness ratio, the phase change temperature, and the thermal conductivity ratio between the thermal insulation layer and phase change material are investigated. The effect of PCM hysteresis on the transient heat transfer process is also evaluated. A pseudo-3D model coupled to the finite difference numerical method is developed to simulate the start-up and shut-in transient processes. To address the liquid and solid states of PCM and their interface, the model for the PCM-matrix composite layer is constituted in the form of enthalpy conservation. The influence of the thermal properties of different matrix and PCM materials on the cooldown time is examined. A lumped parameter model was followed presented for transient thermal analysis of a multilayered subsea pipeline with an intermediate layer embedded with MicroPCMs. The continuous heat transfer processes are simulated, including before, during, and after the phase change. The proposed lumped parameter model is validated by comparison with results by perturbation method and finite difference method.

Prof. Duan is also specialized in tubing hanger of subsea X-trees, metal sealing performance of subsea X-tree wellhead, deepwater collet connector locking mechanism, installation operation of subsea collet connector, sealing structures between subsea connector components, and hub structure design of subsea connectors. Recently, the theoretical design problems of the main parameters of subsea connector's hub structure are detailed in comparison with the shortage of the ASME design method [23]. Therefore, a new analytical model is developed, and named stress analytical method (SAM). The hub structure is separated into two parts, i.e. a thick-walled cylinder and a hollow annular plate, and axisymmetric bending deformation problems of the thick-walled cylinder are proposed. The geometric equations, the constitutive equations, the physical equations, and the equilibrium equations are developed to obtain the analytical displacement solution of the hub structure's thick-walled cylinder. The deformation continuity relationships between the thick-walled cylinder and the hollow annular plate are also established, and the analytical solutions of internal forces, displacements, rotation angles and stress components are obtained accordingly. The accuracy of SAM is investigated by comparing stress calculation results with Finite Element Method (FEM) results. A case study is carried out to compare SAM with ASME design method.

A number of experimental and numerical works of square spudcan of Jack-up rig and

anchor have been conducted [24-31]. Bearing capacity of square spudcan of Jack-up rig based on a three-dimensional failure mode, simplified numerical prediction of the penetration resistance profile of spudcan foundation on sediments with interbeded medium loose layer, on spudcan deep penetration using Eulerian finite element in multi-layer sediments: soil plug mechanism, and prediction the full resistance profile of a spudcan deeply penetrating in dense sand overlying clay based on finite element approach, spudcan footprint interaction in a single soil, Sliding risk of jack-up platform re-installation close to existing footprint and its countermeasure, experimental investigation of jetting effect on spudcan extraction from soft clay, and prediction of anchor penetration depth in clays.

The work related to adhesive joints [32-34] are a mesh-independent technique to evaluate stress singularities in adhesive joints, analytical study of the strength of adhesive joints of riser pipes, and stress analysis of adhesive in a cracked steel plate repaired with CFRP. Applied mathematical and mechanics works [35-37] include a mathematical model for geometric modeling of wire rope strands structure, precise integration method for natural frequencies and mode shapes of ocean risers with elastic boundary conditions and a high-precision curvature constrained Bernoulli-Euler planar beam element for geometrically nonlinear analysis.

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Energy Research at University of Stavanger

by Mohsen Assadi, Member EUAS

Short Biography

Present positions

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

Previous position

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

Education

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

Courses and education

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

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

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

PhD Courses

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

Main fields of competence

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

Project leadership

Mohsen Assadi has been project leader for several nationally financed project in Sweden and Norway as well as several EU-projects.
List of selected projects:

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

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

Prof. Assadi's Energy Research at University of Stavanger

The energy industry is facing tremendous challenges due to the combination of observable impacts of the climate change, ever increasing share of the intermittent renewables in the electricity grid and the uncertainties caused by lack of international consensus concerning the way forward. The multi-dimensional nature of the energy related decisions, affected by economy, technology, policy, social acceptance and more, adds to the complexity of the case. Selection of research activities to provide knowledge and clarity in the current situation is not easy. Conflicting interests from political, economic, social and environmental point of view makes the selection of education programs and research topics difficult for the young generation.

The research activities within the energy research group at University of Stavanger (UiS) have been focused on various aspects of the multi-facetted topic of energy system in transition and its consequences. Given the fact that distributed generation, supported by smart technologies, is foreseen to play a central role in development and transition of the energy systems globally, certain attention was given to R&D activities that can support development of fuel flexible distributed generation technologies to support intermittent renewable energy. The projects listed below are providing an overview over currently ongoing and some recent projects conducted at UiS in support of transition towards carbon neutral energy systems dominated by distributed generation.

Hydrogen

Developing validated component and system models using real plant data has enabled

the research group to carry out system studies for distributed small-scale generation units as well as large scale centralized power plants, utilizing a variety of fuels. Access to validated models provides opportunity for identification of possible system configurations and operational strategies that enable high flexibility, high efficiency and low emissions.
Energy storage and decarbonization of energy intense industries have received considerable attention lately and hydrogen as energy carrier has been pinpointed as the main enabler of the global decarbonization strategy.

Since hydrogen needs to be produced, transported, stored, and finally used, research questions addressing the whole value chain need to be considered from technical, economic, safety and social point of view. The energy group at UiS is currently rebuilding a micro gas turbine based combined heat and power (CHP) unit, utilizing an innovative fuel flexible combustion chamber in collaboration with the German space research center (DLR). The main goal of this project is to investigate use of hydrogen for dispatchable generation in a multi-disciplinary research project, with special focus on use of artificial intelligence (AI) based monitoring and control system for seamless variation of fuel mixture during operation. Providing safe and reliable energy conversion technologies that can support the grid during shortage of renewable generation as well as enabling utilization of green hydrogen, produced during surplus renewable power generation will play a crucial role in realization of carbon neutral energy system.

Considering decarbonization of energy intense industries, where use of renewable electricity for elimination of CO2 emissions in not possible, e.g. steel-, ammonia-, chemical industry, the research work in an ongoing EU project (WWW.ENSYSTRA.EU), has been focused on process modelling where hydrogen has been used to replace carbon-based feedstocks needed in various processes. The models developed enable investigation of techno-economic impact of hydrogen use in these industries. In the light of water scarcity as one of the future global treats, certain efforts have been made to investigate the energy need for water purification and the amount of processed water needed for hydrogen production via electrolysis.

Artificial intelligence-based methods and tools for monitoring and control of energy systems

The current trends towards utilization of data driven modeling (also called digital twins) and artificial intelligence, covering instrumentation, data gathering/storage and data analytics have been the corner stones of the methods and tools developed by the researchers at UiS energy group for the last decade. Data from locally operated units, such as micro gas turbines, internal combustion engines, fuel cells, as well as large-scale commercial power plants have been utilized for optimization of the plant instrumentation and condition monitoring to facilitate predictive and condition based maintenance, enabling higher availability and better plant economy. Access to data driven expert systems for optimum operation and maintenance of an energy systems dominated by distributed generation is essential for successful transition of the current energy systems.

Given the fact that high flexibility, both from fuel and operational point of view, is of outmost importance for security of supply in an energy system dominated by intermittent renewable energy sources, the R&D activities within our energy group have been focused on further development of the real time monitoring capabilities for techno-economic

optimization of carbon free energy conversion and power generation.

Experiences from data driven modeling and research on use of artificial intelligence approaches, based on Artificial Neural Networks (ANN) for optimum operation of distributed generation-based energy systems were further enriched with implementation of smart sensors and automatic data filtering.

The importance of further development of fuel flexible, low emission, small-scale technologies for distributed power generation resulted in establishment of an EU-project, Next Generation Micro Gas Turbines (Next MGT), supported by the Marie Curie program. NextMGT (WWW.NEXTMGT.COM) is financing 15 PhD students from seven partner countries, which focuses on further development and commercialization of the micro gas turbine technology as dispatchable generation option to support the electrical grid of tomorrow dominated by intermittent renewables. All aspects of the technology development from component to system level, as well as the techno-economic aspects of manufacturing and use of this technology are being studied in this project.

Geothermal energy

Stavanger is the petroleum capital of Norway and UiS is recognized for its strong position in petroleum related R&D. Given the fact that there are strong synergies between geothermal energy and petroleum, e.g. geology, drilling, well construction, reservoir modeling, a program area was established at UiS to promote multi-disciplinary collaboration on geothermal energy. These efforts resulted in an EEA-financed project in collaboration with the university AGH-Cracow and the company Muovitech, where various borehole heat exchanger designs will be tested in a pilot setup in Poland and the data extracted will be used for model validation and further optimization of the heat exchanger designs.

Battery technologies

Increased share of intermittent renewable energy, in combination with growth of number of electrical vehicles have increased the demand for batteries. Further development of battery technology for more efficient, cost effective and environmentally friendly batteries is therefore of global interest and a central research area. The energy group at UiS is currently setting up a battery laboratory, lead be Prof. Zhixin Yu, for investigation of manufacturing technologies for batteries in collaboration with the company Beyonder. Material technology, electro chemistry, data driven modeling and analysis are among the research topics that will be studied.

Carbon capture and utilization

CO_2 capture, utilization and storage have been considered as an important measure to realize carbon neutral energy systems.

In and ongoing EEA-financed project, in collaboration with the university AGH-Cracow, CO_2 utilization and storage, used as cushion gas in underground natural gas storage is being investigated. The main idea behind this project is to inject CO_2 in existing geological formations for natural gas storage. The CO_2 will act as compressible gas, enabling storage and reproduction of the natural gas from the geological formation.

Differences in gas density between CO_2 and natural gas will enable injection and reproduction of the natural gas. The research questions in focus of this study are suitable injection positions for minimization of gas mixing, diffusion driven mixing processes, as well as operation optimization of the gas storage unit. Issues related to replacement of natural gas by hydrogen will also be investigated for future development of the gas storage units for hydrogen storage.

A research group at UiS, led by ass. Prof. Mahmoud Khalifeh has recently patented a technology, called safe rock that is providing a carbon free replacement for cement. The preliminary tests have revealed that the safe rock can also absorbed considerable amount of CO_2. A laboratory setup is planned to further investigate the CO_2 utilization capability of the safe rock.

Low temperature heat sources

Utilization of low temperature heat sources and industrial waste heat for heat and power generation has been studied by the UiS energy group to provide better understanding of the economic potential of waste heat utilization. Validated models for waste heat utilization from aluminum industry were developed based on experimental data from test cell setup for system studies and optimization of the design. Currently a heat pump laboratory is under development, utilizing a test rig based on super-critical CO_2 as working fluid. The heat pump will be connected to geothermal wells as well as a flexible heat source to generate experimental data for model validation. AI-based technologies will be used for automated operation and optimization of the unit for seamless variation of the temperature of the heat source.

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Smart High-Performance Microwave Dielectric Ceramics

by Nathan Newman, Member EUAS

Short Biography

Lamonte H. Lawrence Professor in Solid State Science
Arizona State University, Tempe, Arizona 85287-6106

Education

Ph. D.	*Electrical Engineering*	*Stanford University*	*June 1987*
M.S.	*Electrical Engineering*	*Stanford University*	*June 1983*
B.S.	*Biomedical/Electrical Engineering*	*University of Southern Calif.*	*Sept. 1981*

Active Research interests

Materials Science: Synthesis, characterization and modeling of novel semiconductor, superconductor, dielectric, and ferroelectric materials and devices.

Honors , Fellowships and Professional activities

Lamonte H. Lawrence Professor in Solid State Science, Arizona State University, 2009- present.
Member, European Union Academy of Sciences (EUAS), 2020
Fellow, National Academy of Inventors, 2019
Fellow, IEEE, 2013
Fellow, American Physical Society, 2006
Distinguished teaching award, top 5% of teachers in the ASU engineering faculty, 2015
Chair, U.S. Committee for Supercond. Electronics, 2012-2013.
Member, Board of Directors, U.S. Committee for Supercond. Electronics, 2004-present.
Honorary Professor, Amity University, Noida, India, 2014-present.
Van Duzer award, IEEE, 2006
Associate Editor of Materials, IEEE Transactions of Applied Superconductivity 2008-2021
Author or co-author of 230+ articles in archival journals(190), books(6), technical magazines (5) & conference proceedings(29).
9000+ citations and a Hirsch index of 50+
Inventor or co-inventor of 14 U. S. Patents
Editorial board, Journal of Superconductivity and novel magnetism, 2004-2008.
Distinguished teaching award, Electrical Engin. Dept., Northwestern Univ., 1999.
Founding Advisor, Sunrayce solar car undergrad project, Northwestern Univ., 1997-1999.
Coach, 1998 and 1999 seasons and faculty advisor 1997 season, Northwestern Univ. Ice Hockey club team
IBM Fellow, 1984-85, Varian Associates Fellow, 1983-84, summa cum laud, 1981

Professional Experience

Professor, Professor of Materials, Arizona State University (ASU), 3/00-present; Director of the Center of Solid State Science, ASU, 7/06 – 6/2011; Chemical, Bio and Materials Engineering Dept., ASU 3/00 – 6/06, and Interim director of the Center for Solid-State Science, ASU, 7/04 – 6/06. Research focuses on the synthesis, characterization and modeling of novel photovoltaic materials, dilute magnetic semiconductors, superconductors for high field magnet applications, Josephson junctions for 100 GHz+ RSFQ digital logic applications, high-Q microwave dielectrics and ferroelectrics for energy storage applications.
Assoc. Professor, Electrical and Computer Engineering Dept., Northwestern Univ., 3/96 –2/00.
Research focused on the synthesis, characterization and modeling of wide-bandgap photonic semiconductors, high-Q microwave dielectrics, tunable ferroelectrics and adhesion at interfaces.
Scientific Staff Level II, Energy and Environment Div., Lawrence Berkeley Labs, 3/92 to 3/93; Research Staff, Material Science Dept., University of California at Berkeley, 11/91 to 2/96.
Work focused on the development of a fundamental understanding of the thermodynamic and kinetic processes involved in meta-stable growth of GaN using Molecular Beam Epitaxy. The first spectroscopic study was performed which conclusively demonstrated the dominance of point defects (i.e. the AsGa) in the properties of annealed low-temperature GaAs. For the first time, experiments and local density calculations were used to unambiguously prove that Fermi-level pinning at metal/Group III-V semiconductor interfaces is dominated by interfacial defects. Responsible for managing the design & construction of the U. C. Berkeley

Integrated Materials Laboratory, a new facility funded by the National Science Foundation for the growth and characterization of novel thin film structures and devices.
Member of the Technical Staff, Conductus, Inc., Sunnyvale, CA. 94086; 11/88 – 11/91.
Responsible for the growth and characterization of thin-epitaxial layers of high-Tc superconducting films. Through this work, Conductus became one of the leaders in the production of YBa2Cu3O7- films with low-losses and low-noise at microwave frequencies. Responsible for growth of films using off-axis sputtering and for microwave loss measurements using a 11 GHz parallel-plate technique.
Research Assistant: EECS Dept.,Stanford University; 1/83-5/ 87. Advisor: Prof. W. E. Spicer
Research Associate: EECS Dept., Stanford University; 5/87-5/88.
Scientific Staff, Level II: Lawrence Berkeley Labs; 5/87-5/88.
Experiments were initiated to test the possible correlation between the electrical characteristics of thick metal/group III-V Schottky barriers and the chemical and electronic properties of the interface. This work clearly demonstrated a correlation between the near-interfacial As:Ga stroichiometry and the barrier height of GaAs Schottky barriers. This work lead to the development of the widely recognized Advanced Unified Defect Model of Fermi-level pinning at metal/Group III-V semiconductor interfaces.

Abstract
My group's recent work has focused on developing smart microwave dielectric materials. In this review article, I describe how a small (<75 G) magnetic field can be used to switch a low-loss microwave ceramic from a high-Q on-state to a low-Q off-state. This effect can be used to switch high-performance microwave components and subsystems on and off electronically with a small coil. The microwave absorption that induces the lossy low-Q state in the dielectric that we studied, Al_2O_3, is from electron paramagnetic resonant (EPR) transitions in the chosen dopant, an Fe^{3+} ion. While our initial demonstrations were carried out at cryogenic temperatures, I describe our current efforts to achieve similar performance at or near room temperature.

1. Introduction

Over the last few decades, the performance of commercial microwave ceramics has improved to the point that the dielectric resonators and filters used in microwave communication systems now have quality factors greater than 35,000.[1] However, there has been a noticeable absence of any advances to alter their properties electronically. I believe that there will be many practical applications for microwave materials that can be controllably transitioned between a low-loss "on" state and a high-loss "off" state using a magnetic field supplied by a small coil.[2] In one application where multiple microwave systems operate such as on Navy ships[3], the automatic control of the timing of transmission and receive signals could be used to avoid interference between systems. In another application, microwave engineers could use this switching capability to controllably divert microwave signals down different paths to select certain circuit components and/or subsystems at will.

The possibility that we could significantly alter their properties using electronic means came from our studies of commercial high-dielectric-constant temperature-compensated materials.[4-7] While earlier studies had attributed the microwave losses to absorption from anharmonic phonons[8], free carriers [9], and polarons[7,10], we showed that the dominant loss mechanism, at least at low temperatures, is from resonant spin excitations [i.e. electron paramagnetic resonance (EPR) absorption] in unpaired transition metal d-electrons in exchange coupled clusters. [4-5] We went on to suppress the low-temperature EPR losses using large magnetic fields (i.e. >5 T) so that we could quantify the small, but still measurable, loss from polaron hopping conduction between paramagnetic defects.[7] The magnitude of this conduction correlated with the 300 K ambient loss tangent,

suggesting that the defects responsible for carrier conduction play an important role in establishing their performance at room temperature.[7] The observation also clearly showed that we might be able to control the loss tangent in microwave materials with magnetic fields.[2] Making this practical, however, required significant work, as the initial measurements showed that such spin losses are dominant only at very low temperatures and large magnetic fields (~ 2,000-4,000 G) are needed to markedly alter the loss tangent.[4-5] The latter measurements of the magnitude of polaron losses [7] showed what is well known and obvious, that the development of any ceramic material made for practical applications must be of high structural quality and have a small concentration of performance degrading defects.

To reach our goals of achieving higher temperature operation with smaller fields, a basic understanding of electron paramagnetic resonance is required. In order to explain the needed concepts, we show in Figure 1 energy diagrams of prototypical transition-metal paramagnetic ions with one and five electrons in their d-shell. [11] For the $S=^1/_2$ ion, the Zeeman splitting increases with magnetic field, typically resulting in spin absorption (with $\Delta m_L = 0$, $\Delta m_S = 1$) at a field of 2290 G for 6.74 GHz microwaves and 4225 G for 12.44 GHz. Thus, we can rule out this scenario because we desire control at much smaller fields.

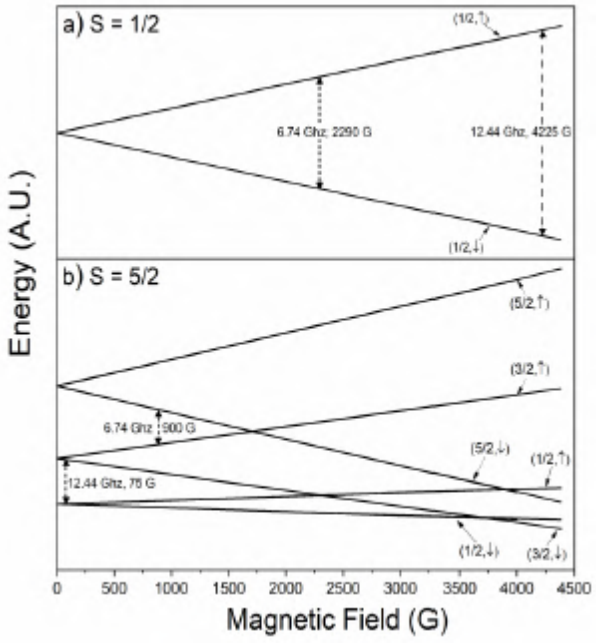

Fig. 4 Schematic energy diagram with the levels labelled as (m_L ,m_S) for (a) $S= {}^1/_2$ showing two energy levels, both with $m_L={}^1/_2$ and (b) $S={}^5/_2$ showing six energy levels, with $m_L={}^1/_2$, ${}^3/_2$ or ${}^5/_2$. For a given m_L, the lower/upper level is for an electron spin in the same/opposing direction with the applied field. The dashed arrows indicate the EPR transitions occuring at the smallest fields for 6.74 GHz and 12.44 GHz microwaves

Next, we analyse a transition ion with 5-d electrons, such as Fe^{3+}, so the d-electrons are half-filled. For this special case, we remember from freshman chemistry that the ion has $S={}^5/_2$, L=0 and $J ={}^5/_2$. From quantum mechanics, the ion has 6 different energy levels, $m_L = \pm ½, \pm {}^3/_2$ and $\pm {}^5/_2$. Note that there is also a component that splits the energies at zero-field which is a result of the small structural displacement in the transition-meal impurity ion from the lattice's centrosymmetric position.[11] The root-cause is the change in the electron's wavefunction (no longer pure d-like) and through the spin-spin and spin-orbit interaction, causes a change in the zero-field energy.[11]. Even if we ignore these details,

we can easily see the very important result that large energy EPR transitions can occur at very small fields.[2, 12]

Before we go on, we point out that a photon has an angular momentum of ± $\hbar$, so the strongest "allowed" transitions are found when $\Delta m_S = \pm 1$ or $\Delta m_L = \pm 1$. Other transitions do occur, but their absorption is typically much smaller in magnitude.

This d^5 configuration is particularly interesting, because ions with half-filled d-electrons (L=0) allow higher temperature operation as a result of a minimal spin-orbit interaction ($L \cdot S$) and corresponding long spin-lattice (T_1) lifetimes. [11] The maximum concentration of isolated transition-metal ions occurs at ~0.5% to 1%.[13] Higher transition-metal doping concentrations result in magnetic exchange interactions between the electrons in the ions, resulting in coupled spin flip absorption in what is labelled as super-spin, and these resonant absorption processes typically occur at undesirably higher magnetic fields[4-5,13].

This review paper describes the methodology that we used to achieve smart microwave ceramics, i.e. materials which can switch back and forth from a low-loss microwave ceramic with a high-Q on-state to a low-Q off-state with a small (<75 G) magnetic field. The results we report are from measurements at reduced temperatures using Fe^{3+} ions in the $(Al_{1-x}Fe_x)_2O_3$ alloy. We will also describe our current approach that we are taking to achieve similar performance at or at least near room temperature.

2. Experimental Methods

$(Al_{1-x}Fe_x)_2O_3$ ceramic samples were synthesized with conventional solid-state powder processing methods using the methods described in reference 2. High-purity Al_2O_3 (99.95%) and Fe_2O_3 (99.95%) powders were dried for 3 h at 100 °C to remove moisture, then ball milled for 1 day in an ethanol aqueous slurry with an addition of 1 wt% stearic acid and 5 wt% paraffin wax binder. The slurry was dried and sieved through a 48-mesh sieve, then pressed. The $(Al_{1-x}Fe_x)_2O_3$ samples were heated at 400 C for 2 h to remove the binder, followed by sintering in air at 1550 °C for 4 hours to a ceramic sample. [2]

Quantitative measurements of the loss tangent as a function of magnetic field were carried out up to ~77 K using a superconductor parallel plate configuration with $YBa_2Cu_3O_{7-\delta}$ superconducting films as the ground planes and an $(Al_{1-x}Fe_x)_2O_3$ plate as the inner dielectric.[14-15] The loss tangents of dielectric materials were measured by inserting the parallel plate resonators into a 2.03 cm x 0.61 cm x 1.52 cm gold-plated copper cavity attached to a cryogenic dipping probe. An HP8510C microwave vector network analyser (Hewlett Packard, Model 8510C) was used to measure S21 vector values using the methods described in Reference [14-15]. These values were then fit to a circle in the Smith chart to determine the unloaded quality factor. Electron paramagnetic resonance transitions were detected by their drop in the loss tangent in the magnetic field sweeps. Additional continuous wave EPR measurements were measured from 4 to 300 K using a commercial EPR X-band microwave bridge system [Bruker, ELEXSYS E580, Silberstreifen, Germany) equipped with an Oxford Model 900 EPL liquid helium cryostat (Oxford Instruments, Oxfordshire, UK). Since the measurements carried out in the commercial Bruker instrument requires a standard to quantify the loss, we only used the signal's relative magnitude under varying temperature and field conditions. Simulations of the electron paramagnetic resonance data were performed using the EasySpin (Model 5.2.15) simulation package. To fit the spectra for the $(Al_{0.9995}Fe_{0.0005})_2O_3$ samples, we used a $S=^5/_2$ spin Hamiltonian with the $R\bar{3}c$ space group symmetry of this alloy system [2].

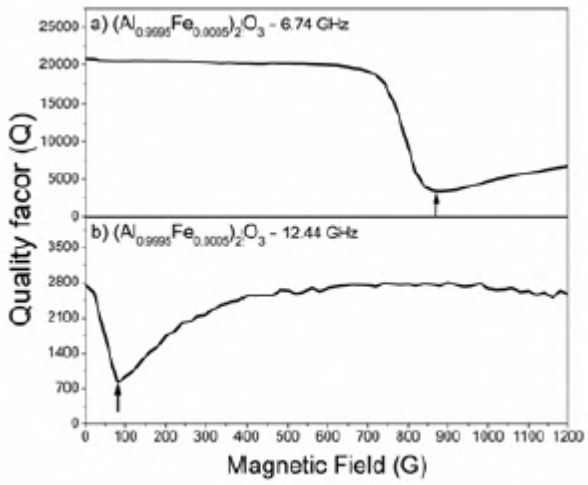

Fig. 5 Quality factor of the fundamental mode of a parallel plate resonator with the $(Al_{0.9995}Fe_{0.0005})_2O_3$ dielectric spacer as a function of applied magnetic field.

3. Results and Discussion

The quality factor of the fundamental mode for the parallel plate resonators at 6.74 GHz and 12.44 GHz measured as a function of magnetic field at 7 K are illustrated in Figure 2a and 2b, respectively. The ability to go from an on-state with a very high quality factor of 21,000 at zero-applied field to a very low of ~3,400 quality factor at ~900 G can be seen in Figure 2a for the relatively lightly-doped $(Al_{0.9995}Fe_{0.0005})_2O_3$ sample. By using a resonator with smaller dimensions, we were able to measure the same lightly-doped $(Al_{0.9995}Fe_{0.0005})_2O_3$ sample at the higher frequency of 12.44 GHz. Since the corresponding photon energy of 51.55 μeV is near the zero-field splitting energy, we see that the low loss state is observed at very small magnetic fields of~75 G, which can easily be accessed with small electromagnetic coils. Since high-performing microwave materials are known to have quality factors that tend to scale inversely with frequency (i.e. constant quality factor x frequency (Qxf) products),[1] we would have expected an on-state quality factors of ~10,000. Such smaller parallel plate resonators have modes that are often limited by radiation-like near-field losses from the nearby gold-plated cavity wall, so we expect that the optimization of the measurement process could achieve similar off-state values, but much higher on-state quality factors greater than 10,000 at frequencies in the 12 GHz range for this material system.

Absorption from spin excitations are found to dominate the loss tangent at low temperatures, but not at higher temperatures as a result of the population redistribution described by the Curie law [16] and the typical marked drop in the T_1 lifetime. However, for systems with L=0 and thus small spin-orbit interactions, the T_1 lifetimes can remain large even up to high temperatures, facilitating observable transitions at room temperature and beyond.[11] Evidence that T_1 did not change markedly comes from the observation that the quality factors in the off-state measured with the commercial Bruker instrument follows reasonably closely to the $^1/_T$ Curie dependence from 4 to 300 K [16]. As can be seen in Figure 2a, the changes in the quality factor of the parallel plate resonator at 7 K is from an on-state value of 21,000 to an off-state value 3,400. The same measurement at 50

K found that the quality factor only switched from 13,000 to 9,000. The relatively high off-state quality factor shows the electron paramagnetic resonant absorption is still strong, but smaller than at the lower temperature. The on-state value was limited to some extent to the $YBa_2Cu_3O_{7-\delta}$ losses and the development of improved measurement techniques that can operate at higher temperatures are in order.

The following approach is planned for the development of materials with improved performance at higher temperatures. First, we need to increase the number of isolated paramagnetic centers to the largest value possible, short of when they would form significant concentrations of exchange coupled pairs and clusters. This optimal concentration falls at about a factor of 20 times greater [13] than we used for this proof-of-concept demonstration. We also will find material where the exchange coupling is over a shorter distance so that a higher density of isolated impurities is possible. We need to do this without significantly broadening the absorption peak and without inducing other parasitic losses, like impurity-mediated electron hopping. Computer simulations of dipole broadening in the presence of exchange coupling are needed. The model's parameters for conventional material are known, but experiments are still needed to acquire them for the newer practical high dielectric-constant (>25) microwave ceramics. Although density functional calculations are not accurate enough to provide the needed precision, we can use them to predict useful trends and guide the experiments. Also, new host materials are needed that have excellent dielectric properties and lattice configurations that facilitate higher paramagnetic doping concentrations that minimize the coupling that results in exchange coupled pairs and higher complexes. Initial work toward this goal is described in Reference 17.

4. Conclusions

To summarize, in this study, we have uncovered a method that can convert a low-loss material, with a high quality factor, into a high-loss material, with a low quality factor, through the application of a small magnetic field. A few potential applications would include the ability to switch high-performance microwave components and subsystems on and off electronically with a small coil. We have outlined a plan to continue to optimize the material properties so that high-Q switchable devices should be able to operate above 77 K.

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Design of Aircraft Control Systems, Aerospace Control Applications, Engineering Automatic Feedback Controllers & Robotics

by Frank Lewis, Member EUAS

Short Biography

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

Ranked at position 89 worldwide, 64 in the USA, and 3 in Texas of all scientists in Computer Science and Electronics, by Guide2Research. Fellow, National Academy of Inventors. Fellow of the IEEE, Fellow of IFAC, Fellow of the U.K. Institute of Measurement & Control, Fellow American Association for the Advancement of Sciences, Member of the New York Academy of Sciences. Registered Professional Engineer in the State of Texas and Chartered Engineer, U.K. Engineering Council. 68,500 google citations, h-index 116. Charter Member (2004) of the UTA Academy of Distinguished Scholars. UTA Academy of Distinguished Teachers 2012. IEEE Control Systems Society Distinguished Lecturer 2012-1014. Founding Member of the Board of Governors of the Mediterranean Control Association. Served as Visiting Professor at Democritus University in Greece, Hong Kong University of Science and Technology, Bristol University UK, Chinese University of Hong Kong, City University of Hong Kong, National University of Singapore, Nanyang Technological University Singapore.

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

Texas Regents Outstanding Teaching Award 2013.
Current interests include autonomous systems, unmanned aerial vehicles, distributed cooperative control on graphs, reinforcement learning, nonlinear systems, intelligent control, process control, and neurobiological systems. Author of 7 U.S. patents, 420 journal papers, 52 chapters and encyclopedia articles, 420 refereed conference papers, and 20 books including Optimal Control, Optimal Estimation, Applied Optimal Control and Estimation, Aircraft Control and Simulation, Control of Robot Manipulators, Neural Network Control, High-Level Feedback Control with Neural Networks and the IEEE reprint volume Robot Control. Editor of Taylor & Francis Book Series on Automation & Control Engineering. Served as Editor for the flagship journal Automatica. Served/serves on many Editorial Boards including International Journal of Control, Neural Computing and Applications, Optimal Control & Methods, and Int. J. Intelligent Control Systems. Recipient of NSF Research Initiation Grant and continuously funded by NSF since 1982. He has received $12 million in funding from NSF, ARO, ONR, AFOSR and other government agencies, including significant DoD SBIR and industry funding. His SBIR program was instrumental in ARRI's receipt of the US SBA Tibbets Award in 1996.

Accomplishments

Dr. Lewis has made fundamental contributions in the design of aircraft control systems, aerospace control applications, engineering automatic feedback controllers, robotics, and unmanned systems technologies since 1983. During 1983-1987 he developed a new unified design methodology for Optimal Control of aircraft autopilots and feedback control systems while consulting at Lockheed Advanced Research Organization. He is internationally known for his resulting textbook "*Aircraft Control and Simulation*" (1992, 2003) which, along with his other texts, has influenced numerous control engineers over three decades.

Lewis developed during the 1990s a new generation of nonlinear adaptive feedback controller structures with significantly improved performance for intelligent flight control and nonlinear dynamic systems. The essential contributions of his technology were to invent novel closed-loop feedback structures and parameter tuning laws that combine adaptive control robustifying terms and backpropagation tuning using nonlinear function approximation methods.

He provided a fundamental breakthrough by developing new rigorous mathematical analysis and proof techniques that provide learning of unknown nonlinear dynamics as well as guaranteed closed-loop performance and stability as required by Mil-Spec. His analysis proof techniques changed the technical outlook of the field and are now in common use in high performance nonlinear adaptive control systems. This technology led to 4 US patents. Lewis published profusely and wrote the first textbooks in neural adaptive control. His work is highly cited and started an extensive new literature in rigorous design techniques for nonlinear neural adaptive control systems.

For these innovations, Lewis was elected a Fellow of the National Academy of Inventors (NAI) and received the 2016 AIAA Intelligent Systems Award and other

top awards from various IEEE societies. He is currently listed as number 88 worldwide and 66 in USA of all Scientists in Computer Engineering and Electronics by http://www.guide2research.com/scientists/.

Impact

Lewis' accomplishments led to 7 US patents and significant technology transition to US industry. Scientists at Boeing Defense Space and Security Systems used Lewis' novel adaptive control technology of 1999 Patent 5,943,660 to develop more effective and highly reliable adaptive uncertainty approximation compensators for flight control application in their unmanned aircraft and advanced weapon systems. These adaptive flight control systems are flown in the Phantom Ray unmanned aircraft which has been fielded for defense by the US Army.

Researchers at Georgia Tech used dynamic inversion to extend Lewis' 2003 Patent 6,611,823 to develop flight control architectures and tuning algorithms for improved control of unmanned aerial vehicles. Aircraft autopilots based on this technology are marketed by Guided Systems Technology, Inc.

Lewis' student Jagannathan extended the technology of 2000 Patent 6,064,997 and US Patent 9,134,707 to develop under industry contract Optimal auto engine controllers for Caterpillar, Ford (Zetec engine), and GM, demonstrating 8-10% improvement in fuel efficiency and a drastic reduction in NOx (90%) and HC (30%). Savings to Caterpillar were over $65,000 per unit.

In further Commercial Impact, Dr. Lewis transferred technology to U.S. small companies in flexible vehicle systems, sensor processing, intelligent diagnostics, and automobile suspension systems. He received numerous SBIR contracts with Simis Labs, Sagent Corp., Intelligent Automation, Davis Technologies, Signal Processing, Inc. He was a key contributor to the receipt by his institution of the 1996 U.S. SBA SBIR Tibbets Award. He was listed in Ft. Worth Business Press, Who's Who in Manufacturing, Top 200 Leaders, 1999.

Dr Lewis has graduated 52 PhD students who have had societal impact including President, Istanbul Bogaziki University; President, Univ. New Mexico; and Vice-Chancellor, Univ. Hawaii System. Many of his students now work at high levels in US industry

Evaluation of a Portable Nanopore-based Sequencer for Detection of Viruses in Water

by Joan Rose, Member EUAS

Short Biography

Dr. Joan Rose serves as the Homer Nowlin Chair in Water Research at Michigan State University, the Co-Director of the Center for Advancing Microbial Risk Assessment (CAMRA) a 10 million dollar grant funded by the EPA and US Department of Homeland Security. She is also the Director of the Center for Water Sciences (CWS). Dr. Rose received her B.S., in 1976 from University of Arizona, her MS from University of Wyoming in 1980 and Ph.D. in Microbiology from the University of Arizona in 1985. She served as a Professor in the College of Marine Science, University of South Florida (USF) from 1998-2002 and Associate Professor, Department of Marine Science, USF from 1994-1997. In 1995, she was an Assistant Professor, Department of Environmental and Occupational Health, USF, and from 1986-1989, she served as Research Associate/Lecturer, Department of Microbiology and Immunology, UAZ.

Dr. Rose is an international expert in water microbiology, water quality and public health safety publishing more than 300 manuscripts. She has been involved in the investigation of numerous waterborne outbreaks world-wide. Her work has examined new molecular methods for waterborne pathogens and zoonotic agents such as Cryptosporidium and enteric viruses and source tracking techniques. She has been involved in the study of water supplies, water used for food production, and coastal environments as well as water treatment wastewater treatment, reclaimed water and water reuse and quantitative microbial risk assessment. She specifically interested in microbial pathogen transport in coastal systems and has studied the impact of wastewater discharges and climate on water quality. She was named as one of the 21 most influential people in Water in the 21st Century by Water Technology Magazine in 2000 and won the Clarke Water Prize ($50,000. prize) (one of 5 international awards for contributions to water science and technology).

She current serves on a number of advisory committees include 1) Chair of the Drinking Water Committee for the Science Advisory Board for the U.S. Environmental Protection Agency 2) Vice-Chair of USA National Committee for the International Water Association, 2002-05, 4) Member of the Strategic Council for IWA 2005-08, 3) Chair of the Specialist Group Health-Related Water Microbiology (IWA). 4) She is currently advisory to the Governments of Singapore and Queensland, Australia, serving as chair of the audit committee for the Public Utilities Board in Singapore for the last 4 years.

She was appointed to Water Science and Technology Board of National Academy of Science, National Research Council, 1998-2004 and served as Vice Chair of the Board from 2002-04. Professional society memberships include American Academy of Microbiologists, American Public Health Association, American Society of Microbiology,, American Water Works Association (AWWA), Society for Risk Analysis, International Water Assoc. and Water Environment Federation.

Sources of recent grant and/or contract support include NOAA, EPA, Water Environ. Research Foundation, and NSF,

Positions and Honors

Positions and Employment

1986-1989: Research Associate/Lecturer, Department of Microbiology and Immunology, and Nutrition and Food Science, University of Arizona

1989-1994: Assistant Professor, Department of Environmental and Occupational Health, University of South Florida

1994-1997: Associate Professor, Department of Marine Science, University of South Florida

1995: Courtesy Appointment, Associate Professor, Department of Civil and

Environmental Engineering, University of South Florida
1998-2002: Professor, College of Marine Science, University of South Florida
2005-2014: Co-Director, Center for Advancing Microbial Risk Assessment (CAMRA), Michigan State University (Center of Excellence DHS/EPA)
2003-present: Homer Nowlin Endowed Chair for Water Research, Michigan State University
***Honors** (Most Recent)*
Member of the National Academy of Engineering, inducted 2011
Awarded the KWR Water Fellow, Netherlands, October, 2016
Stockholm Water Prize 2016
Recipient of The Michigan Environmental Council's Helen & William Milliken Distinguished Service Award, 2018

Ji, P.; Aw, T.G,; Van Bonn, W. and Rose, JB. 2020. Evaluation of a portable nanopore-based sequencer for detection of viruses in water. J. of Virol Methods Vol 278:113805.

Abstract

The newly emerged nanopore sequencing technology such as MinION™ allows for real-time detection of long DNA/RNA fragments on a portable device, yet few have examined its performance for environmental viromes. Here we seeded one RNA virus bacteriophage MS2 and one DNA virus bacteriophage PhiX174 into 10 L well water at three levels ranging from 1 to 21,100 plaque-forming units (PFU)/mL. Two workflows were established to maximize the number of sequencing reads of RNA and DNA viruses using MinION™. With dead-end ultrafiltration, PEG precipitation, and random amplification, MinION™ was capable of detecting MS2 at 155 PFU/mL and PhiX174 at 1–2 PFU/mL. While the DNA workflow only detected PhiX174, the RNA workflow detected both MS2 and PhiX174. The virus concentration, or relative abundance of viral nucleic acids in total nucleic acids, is critical to the proportion of viral reads in sequencing results. Our findings also highlight the importance of including control samples in sequencing runs for environmental water samples with low virus abundance.

Kiulia, N.M., Gonzalez, R., Thompson, H., Aw., T.G., and Rose, J.B. 2020. Quantification and Trends of Rotavirus and Enterovirus in Untreated Sewage Using Reverse Transcription Droplet Digital PCR. *Food and Environmental Virology*, In Press

Abstract

The quantification and trends in concentrations for naturally occurring rotaviruses (RV) and enteroviruses (EV) in untreated sewage in various wastewater systems have not often been compared. There is now greater interest in monitoring the infections in the community including live vaccine efficacy by evaluating untreated sewage. The goals of this study were to 1) survey the concentrations of naturally occurring RV and EV in untreated sewage using a reverse transcription—droplet digital polymerase chain reaction (RT-ddPCR) and 2) investigate the use of a new adsorption elution (bag-mediated filtration system (BMFS) using ViroCap filters) against more traditional polyethylene glycol (PEG)

precipitation for virus concentration. Sewage samples were collected from lagoons in Kenya and Michigan (MI), the United States (USA) and from wastewater treatment plants (WWTPs) in the USA. RVs were detected at geometric mean concentrations in various locations, California (CA) 1.31 × 105 genome copies/L (gc/L), Kenya (KE) 2.71 × 104 gc/L and Virginia (VA) 1.48 × 105 gc/L, and EVs geometric means were 3.72 × 106 gc/L (CA), 1.18 × 104 gc/L (Kenya), and 6.18 × 103 gc/L (VA). The mean RV concentrations using BMFS-ViroCap in split samples compared to PEG precipitation methods demonstrated that the levels were only 9% (#s BMFS/PEG) in the Michigan lagoons which was significantly different ($p < 0.01$). This suggests that RV concentrations in Kenya are around 1.69 × 106 gc/L. Overall, there was no difference in concentrations for the other sampling locations across the methods of virus recovery (i.e., PEG precipitation and HA filters) using one-way ANOVA ($F = 1.7$, $p = 0.2739$) or Tukey–Kramer pairwise comparisons ($p > 0.05$). This study provides useful data on RV and EV concentrations in untreated sewage in Kenya and the USA. It also highlights on the usefulness of the RT-ddPCR for absolute quantification of RV and EV in sewage samples. The BMFS using ViroCap filters while less efficient compared to the more traditional PEG precipitation method was able to recover RVs and EVs in untreated sewage and may be useful in poor resource settings while underestimating viruses by 1 to 1.5 logs.

Kitajimaa, M., Ahmed, W. Bibby, K., Carducci, A. Gerba, C.P., Hamilton, K.A., Haramoto,E. and Rose, J.B. 2020. SARS-CoV-2 in wastewater: State of the knowledge and research needs. ***Science of the Total Environment*****: 739:(139076) 1-19.**

Abstract

The ongoing global pandemic of coronavirus disease 2019 (COVID-19) caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has been a Public Health Emergency of International Concern, which was officially declared by the World Health Organization. SARS-CoV-2 is a member of the family *Coronaviridae* that consists of a group of enveloped viruses with single-stranded RNA genome, which cause diseases ranging from common colds to acute respiratory distress syndrome. Although the major transmission routes of SARS-CoV-2 are inhalation of aerosol/droplet and person-to-person contact, currently available evidence indicates that the viral RNA is present in wastewater, suggesting the need to better understand wastewater as potential sources of epidemiological data and human health risks. Here, we review the current knowledge related to the potential of wastewater surveillance to understand the epidemiology of COVID-19, methodologies for the detection and quantification of SARS-CoV-2 in wastewater, and information relevant for human health risk assessment of SARS-CoV-2. There has been growing evidence of gastrointestinal symptoms caused by SARS-CoV-2 infections and the presence of viral RNA not only in feces of infected individuals but also in wastewater. One of the major challenges in SARS-CoV-2 detection/quantification in wastewater samples is the lack of an optimized and standardized protocol. Currently available data are also limited for conducting a quantitative microbial risk assessment (QMRA) for SARS-CoV-2 exposure pathways. However, modeling-based approaches have a potential role to play in reducing the impact of the ongoing COVID-19 outbreak. Furthermore, QMRA parameters obtained from previous studies on relevant respiratory

viruses help to inform risk assessments of SARS-CoV-2. Our understanding on the potential role of wastewater in SARS-CoV-2 transmission is largely limited by knowledge gaps in its occurrence, persistence, and removal in wastewater. There is an urgent need for further research to establish methodologies for wastewater surveillance and understand the implications of the presence of SARS-CoV-2 in wastewater.

Bivens et al 2020. Wastewater-Based Epidemiology: Global Collaborative to Maximize Contributions in the Fight Against COVID-19. *Environ. Sci. Technol. 54*, 13, 7754–7757 Publication Date: June 12, 2020

View Point

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), a novel member of the *Coronaviridae* family, has been identified as the etiologic agent of an ongoing pandemic of severe pneumonia known as COVID-19. To date there have been millions of cases of COVID-19 diagnosed in 184 countries with case fatality rates ranging from 1.8% in Germany to 12.5% in Italy. Limited diagnostic testing capacity and asymptomatic and oligosymptomatic infections result in significant uncertainty in the estimated extent of SARS-CoV-2 infection. Recent reports have documented that infection with SARS-CoV-2 is accompanied by persistent shedding of virus RNA in feces in 27% to 89% of patients at densities from 0.8 to 7.5 $\log_{10}$ gene copies per gram. The presence of SARS-CoV-2 RNA in feces raises the potential to survey sewage for virus RNA to inform epidemiological monitoring of COVID-19, which we refer to as wastewater-based epidemiology (WBE), but is also known as environmental surveillance.

Several studies have reported the detection of SARS-CoV-2 RNA in wastewater in the early stages of local outbreaks, further supporting the technical viability of WBE. WBE could be especially informative given that asymptomatic and oligosymptomatic infections are unlikely to be detected during clinical surveillance. In such instances, WBE can be used to determine the burden of undiagnosed infections at the population level, which is critical to refining estimates of case-fatality rates. Additionally, wastewater offers an aggregate sample from an entire community that is more easily accessible than pooled clinical samples. Along with clinical data and other technological approaches, such as contact tracing, WBE could provide critical monitoring of SARS-CoV-2 transmission within a community including the beginning, tapering, or re-emergence of an epidemic. This approach mirrors previous efforts in environmental monitoring, for example poliovirus RNA, to inform mechanistic models of pathogen transmission dynamics.

Chen, C.; Örmeci, B.; Rose, J.B.; Thanikal, J.V; Hayward, K.; Khan, S. J.; Pillay, S. and Zhang, T. 2020 The Role of Wastewater Treatment in COVID-19 Control, *Water Quality Research Journal of Canada*

Abstract

The International Water Association (IWA) initiated a Task Force in April 2020 to serve as a leadership team within IWA whose role is to keep abreast and communicate the

emerging science, technology, and applications for understanding the impact and the ability to respond to the COVID-19 pandemic and specifically designed for water professionals and industries. Expertise was nominated across the world with the purpose of collectively providing the water sector with knowledge products for the guidance on the control of COVID-19 and other viruses. This review paper developed by a working group of the IWA Task Force focuses on the control of COVID-19. The purpose of this review paper is to provide an understanding of existing knowledge with regards to COVID-19 and provide the necessary guidance of risk mitigation based on currently available knowledge of viruses in wastewater. This review paper considered various scenarios for both the developed world and the developing world and provided recommendations for managing risk. The review paper serves to pool the knowledge with regards to the pandemic and in relation to other viruses. The IWA Task Team envisage that this review paper provides the necessary guidance to the global response to the ongoing pandemic.

Drug Formulations Science Research

by Mansoor A. Khan, Member EUAS

Short Biography

Dr. Mansoor A. Khan has served FDA for over 11 years as the Director of Product Quality Research and a Senior Biomedical Research Scientist (SBRS) at CDER, where he helped develop regulatory policies for reviews and compliance, and led cmc review and research teams on drug delivery systems, product stability, biotech products, and biopharmaceutics. In Sept of 2015, he joined Texas A&M University as Professor and Vice Dean at the Rangel College of Pharmacy in College Station, TX. Prior to joining FDA in 2004, Dr. Khan was a Professor of Pharmaceutics and Director of Graduate Program in the School of Pharmacy at Texas Tech University Health Science Center. He earned his Ph.D. degree in Industrial Pharmacy from the St. John's University School of Pharmacy at New York in 1992. He has published over 325 peer-reviewed manuscripts, five texts including "Quality by Design for Biopharmaceutical Drug Product Development, 30 book chapters, 250 poster presentations, and more than 275 invited presentations world-wide.

Dr. Khan has held several leadership positions at the American Association of Pharmaceutical Scientists (AAPS) including elected chair of pharmaceutics and drug delivery (PDD) and the founding chair of formulations design and development (FDD). He serves on the editorial board of Pharmaceutical Technology, International Journal of Pharmaceutics, AAPSPharmsciTech, and Drug Delivery and Translational Research. As a formulations expert, Dr. Khan served as a FDA representative to EMA/PDCO, WHO, USP, NIH, DoD, DARPA, NASA, and Bill and Melinda Gates Foundation. He also served as the science policy advisor to CDER Center Director where he helped resolve complex issues of drug reviews and compliance with science. He has also led the chemistry review team that approved the first 3D printed tablets in August 2015. Dr. Khan has received outstanding alumni award from St. Johns University, College of Phamacy, Excellence Award from Texas A&M University Health Science Center, over fifteen FDA/CDER Team Excellence Awards, FDA/CDER Scientific Achievement Award, and FDA/CDER Exemplary Performance Awards. Additionally he received the AAPS Research Achievement Award in Formulations Design and Development. He is also an AAPS and AAiPS Fellow.

Drug formulations science research in our laboratory is focused on premarket development of novel dosage forms and delivery systems including pediatric medications and 3D printed products, modified release dosage forms, complex generic product development for oral, topical/transdermal and ocular delivery systems, quality by design with process analytical technologies, and post-market research to identify the root cause of products failures and safety issues of narrow therapeutic index drugs.

I have contributed significantly on the advancement of pharmaceutical science. My research focused on formulation and process development, process monitoring, manufacturing, 3D printed dosage forms, narrow therapeutic index drugs quality and safety, pediatric dosage forms, quality by design and process analytical technologies, modified release dosage forms, transdermal and ocular delivery system etc.

Children require different oral dosage forms than adults due to differences in swallowing abilities, taste preferences, and dosage requirements. Most medications are produced for adults as capsules and tablets, which are often not suitable for children. Drugs prescribed to children have historically been those that were approved for and prescribed to adult patients, although they were rarely testing in the pediatric subpopulation. As a result, over 80% of product labeling did not provide directions for safe and effective use in pediatric patients. However, pediatric formulations are available for few drugs, most of

these formulations are not taste masked. The lack of availability of pediatric friendly formulations is primarily due to evolving physiological and pharmacogenetic development of children where fixed doses do not work. Physicians or patient care providers have no choice but to prescribe the dosage forms, which are intended for adults and often times, unpalatable. Children commonly refuse to take medications if it tastes bad. This results in lack of adherence and can lead to hospital admissions for intravenous therapy. Often, the physicians prescribe extemporaneous preparation where drug product is manipulated in pharmacy with a goal to adjust dose of the drug due to unavailability of lower strength of the product, not to make drug product children friendly. However, concerns are raised by physician and FDA alike on lack of dose accuracy, stability/sterility, pharmacokinetic/pharmacodynamics studies, efficacy and safety, and consistency in preparation of extemporaneous preparations. From the pediatricians' perspective, the availability of easy to swallow and palatable formulations of pediatric friendly can mean the difference between treatment success and failure. An ideal pediatric product of anticancer drug should have ability to titrate dose (dose flexibility) so that wide age group (0-17) of children can be covered by a single product which is easy to swallow/dissolvable form, palatable, contains minimal/safe excipients, has adequate bioavailability and is stable at high heat and humidity etc. I have promoted development of pediatric friendly dosage through policy, regulation, and research. I have worked on various technologies to develop pediatric friendly dosage forms e.g. complexation, co-crystals, salts engineering, coating, novel dosage forms etc. I have presented on FDA policy and regulation, and approaches to develop pediatric dosage forms in federal agencies, and national and internal conferences e.g. AAPS, EUPFI, DIA, FDA, NIH, etc.[1-13]

Three dimensional (3D) printing or additive manufacturing is the 21st century manufacturing technology. Unlike traditional manufacturing methods (subtractive manufacturing) which involve assembling parts in an assembly line to make an end-user product, 3D printing technology involves the process of making 3D objects by layering down successive layers of material until the object is created from a digital file of computer aided design under the control of computer software. It has enormous potential across industries, and one of the most transformative applications has been in the medical field including personalized medical devices and drug products. FDA has approved about eighty-five 3D printed medical devices through 510(K) process, and just one drug product, Spritam®. It is manufactured by ZipDose® technology, where the dosage form disintegrates in few seconds. Spritam® contains high dose (250-1000 mg) of the drug and disintegrate very rapidly (mean disintegration time is about 11 sec in mouth), which is ideal for patients with swallowing difficulties. In FDA, I led team of scientists and reviewers for approval of Spiritam®. Currently, we are working on 3D printing technologies (selective laser sintering and fused deposition modeling) for the development of dosage forms for compounding of personalized medications especially, geriatric, pediatric and special population who are sensitive to components of commercial formulations (lactose intolerance or allergic to dye or other excipients etc.). We have published many review and research papers on 3D printing of pharmaceuticals in peer reviewed journals.[14-19]

Research in our laboratory also includes quality by design (QbD) and process analytical technology (PAT) in pharmaceutical development and manufacturing. FDA encourages risk-based approaches and the adoption of QbD principles in drug product development, manufacturing, and regulation. FDA's emphasis on QbD began with the recognition that increased testing does not necessarily improve product quality. Quality must be built into the product. Pharmaceutical QbD is a systematic approach to development that begins with predefined objectives and emphasizes product and process understanding and control based

on sound science and quality risk management. QbD consist of following elements: quality target product profile that identifies the critical quality attributes; product design and understanding including the identification of critical material attributes; process design and understanding including the identification of critical process parameters and a thorough understanding of scale-up principles; a control strategy that includes specifications for the drug substance(s), excipient(s), and drug product as well as controls for each step of the manufacturing process and process capability and continual improvement. Implementation of QbD involved use of statistical method and process monitoring. Statistical methods such as multivariate analysis and design of experiments to understand formulation and process variables. PAT is a mechanism to design, analyze, and control pharmaceutical manufacturing processes through the measurement of critical process parameters which affect critical quality attributes. It ensures that the process remains within an established design space and provide continuous monitoring of critical process parameters, critical material attributes, or critical quality attributes to make go/no go decisions and to demonstrate that the process is maintained in the design space. We have extensively used statistical methods to understand and develop process and formulation e.g. coprecipitation, encapsulation, niosomes, microparticles, nanoparticles, liposomes, freeze-drying process, granulation, ointment, cream etc. We have used Focused beam reflectance measurement, THz spectroscopy, near infrared, particles-vision monitoring, FTIR probes as a PAT to understand, monitor and control various pharmaceutical manufacturing process.[20-46]

Transdermal drug delivery systems (TDDS), also known as “patches,” are dosage forms designed to deliver a therapeutically effective amount of drug across a patient’s skin. Several TDDS containing drugs such as clonidine, estradiol, fentanyl, nicotine, nitroglycerin, oxybutynin and scopoloamine are available in the United States. Quality issues reported for TDDS are adhesion lacking, cold flow, crystallization etc. Various approved TDDS have been recalled due to quality failure that may affect safety and efficacy of drug product. We have addressed root cause of quality issues and developed and standardized methods to quantify cold flow. Cold flow is analogous to drug leakage from the edge of membrane-controlled TDDS is one of the product quality defects associated with drug-in-adhesive (DIA) type of TDDS. The liquid excipient(s) and drug(s) plasticize pressure-sensitive adhesives (PSA) of DIA-TDDS to varying degree depending on their physicochemical properties and composition. Imbalance in the degree of PSA plasticization may result in oozing out (creeping) of DIA from under the backing membrane beyond the edge of TDDS (cold flow) leading to storage problems, adhesion failures and formation of dark ring on application to skin. Cold flow was induced by applying 1 kg weight to patch stored at 25°C, 32°C, and 40°C/60%. Cold flow induced at 32°C/60%RH in 2 days with 1 kg force is clinically relevant and can be used to assess susceptibility of the TDDS to cold flow. We also developed stereomicroscopic imaging technique to quantify the cold flow. Other aspects of TDDS studied were skin-skin drug transfer for safety of potent drug (fentanyl, estradiol etc) and development of in-vitro and in-vivo correlation that can be used to predict performance of past-marketed change in the product.[47-50]

The generic pharmaceutical drug products have to conform to the same standards of quality, efficacy, and safety requirement of innovator drug products. Testing procedures are to be established to prove that generic pharmaceutical drug products are therapeutically equivalent and interchangeable with their associated innovator’s product. The regulation 21 CFR 320.24(b) provides a list of in vivo and in vitro methods to establish bioequivalence in descending order of preference: (i) in vivo studies in humans comparing drug/metabolite concentrations in an accessible biological fluid, (ii) in vivo testing in

humans of an acute pharmacological effect, (iii) controlled clinical trials in humans to establish safety and efficacy, (iv) in vitro methods, and (v) any other approach deemed adequate by FDA. One or more of these approaches might be used to demonstrate bioequivalence (BE). For example, the bioequivalence of solid oral dosage forms intended for systemic delivery is established by in vivo pharmacokinetic (PK) studies with a support of comparative in vitro dissolution data. This approach has been successfully applied to a large number of drug products. However, the conventional in vivo BE study with PK end points such as C_{max} and AUC is neither appropriate nor feasible for testing the potency of topically applied ophthalmic cyclosporine microemulsion. Determination of bioequivalence of locally acting drugs in the eye is more complicated as local drug concentrations cannot be measured directly. Therefore, it is a challenging issue for both the pharmaceutical industry and the regulatory agency to determine the BE of locally acting drugs in the eye. We have developed in-vitro quality approach for cyclosporine ophthalmic emulsion and acyclovir ocular ointment as an alternative to in-vivo BE testing for ocular drug product which form the basis for the approval of generic version of brand drug products. We have published our research work in *Molecular Pharmaceutics* and *International Journal of Pharmaceutics*. FDA awarded team excellence award for developing a performance matrix for equivalence evaluation of cyclosporine ophthalmic emulsions, paving the pathway for generic approvals, and provided scientific support to address sponsors' citizen petition.[51-54]

Poor bioavailability is a major challenge to formulate an oral dosage form. Poor aqueous solubility is one of the important underlying factors of bioavailability because a drug cannot be absorbed through the gastrointestinal tract unless it is in solution state. Many chemical entities with significant and promising pharmacological effect suffer from poor aqueous solubility. It is stated earlier that over 30% of the most commonly marketed drug and nearly half of the new drug entities reaching to the formulation scientists are hydrophobic in nature or lacking required aqueous solubility. Several approaches have been adopted to improve the drug solubility and absorption such as modification of crystal habit, reduction of particle size, solid dispersions, solid solutions, salt formation, and miscellaneous methods, including supercritical fluid process and use of surfactant, solubilizers, cosolvency, hydrotrophy, and novel excipients as adjuvant to increase solubility. Lipid-based drug delivery system has gained major attention in the past few decades with the target of bioavailability enhancement of poor water soluble or lipophilic drug administered orally. The main idea of this type of formulation is to keep the lipophilic drugs in dissolved state as a colloidal dispersion throughout the gastrointestinal tract. Self-nanoemulsifying drug delivery systems (SNEDDS) is a lipid-based drug delivery that emulsify in nano-sized droplets in the gastrointestinal tract. We have developed SNEDDS of all trans retinol and ubiquinone to enhance their oral bioavailability for oral absorption. We have encased in capsule/tablet dosage forms for ease of manufacturing and administration.[55-63]

Narrow therapeutic index (NTI) drugs comprise of products where small differences in dose or blood concentration may lead to serious therapeutic failures and/or adverse drug reactions that are life-threatening or result in persistent or significant disability or incapacity. Examples of NTI drugs that we have addressed quality issues are warfarin, phenytoin sodium, tacrolimus, and theophylline. Phenytoin is a first line drug for generalized tonic-clonic epileptic seizure. FDA approved it 1953 for clinical use. Commercially, it is available as a chewable tablet, suspension, and extended release capsule, which contains either phenytoin or phenytoin sodium (PS). The generics differ from the brand as well among themselves in terms of the composition of inactive

ingredients (qualitative and quantitative), manufacturing method, processing parameters, in-process control, specifications, and container closure etc. This may be manifested in clinical performance when a product switch to another. Furthermore, differences in products clinical performances are not only because of inherent properties of the drug but may also be due to quality differences among products. This is further evident from field alert reports (FAR). PS products is among the top ten drugs that have been recalled by FDA due to its failure to meet quality specifications in the field alert reports. Brand and generics products of extended PS capsule have been recalled in the past due to quality failure. We started research on phenytoin to find out sources of quality variation and possible impact on clinical outcome. We thoroughly performed the investigation to understand excipients, process, and stability interplay on the critical quality attributes of PS extended release capsule. Our studies indicated significant effect of excipient, process variables and stability on the critical quality attributes of PS extended release capsule that has potential impact on the clinical performance of the product. For the first time, we were able to figure out major source of quality variation in PS capsules. It was due to the presence of lactose which dramatically changes the quality. Exposure to high humidity causes conversion of PS to phenytoin base and chemical reaction between the drug and lactose. This causes significant reduction in dissolution. To test the hypothesis, we also tested commercial products containing lactose and without lactose. Lactose containing commercial product failed to meet pharmacopeial dissolution and impurity specifications. We have published our findings in *International Journal of Pharmaceutics, Journal of Pharmaceutical Sciences* and *AAPS PharmSciTech*.[64-67]

Warfarin sodium (WS) also belongs to NTI drug that requires frequent monitoring of prothrombin time. Despite its NTI category, product quality plays a pivotal role in minimizing fluctuation in the plasma level. WS absorption occurs mostly in stomach and proximal region of the intestine, however, if the drug product fails to disintegrate/dissolve in the upper gastrointestinal tract due to poor product quality (change to gluey forms), patients may get a subtherapeutic dose. The brand product of WS contains crystalline forms while some of the generic products contain amorphous form. Patients often exhibit clinical variability when they are switched from brand to generic of WS. This substitution has caused some patients to be hospitalized. This variability in clinical outcome might be due to differences in product quality of WS or change in product quality during shelf life. We worked extensively in FDA laboratories on various quality issues of WS and published five research papers in high impact journals. We showed that WS product quality changes when a crystalline phase of WS changes to amorphous gluey-phase due to incorrect manufacturing and processing method, excipients, packaging or exposure to high humidity and temperature conditions. This results in an increase in hardness, disintegration time and slow dissolution rate, which may have ramifications on its oral absorption. We have published six papers on various quality aspects of WS.[68-73]

Commercially available formulations of tacrolimus are the amorphous solid dispersion (ASD) intended to improve its dissolution rate and bioavailability. As with any amorphous drug form, it is intrinsically unstable and reverts to its stable forms. The conversions are even faster if not formulated or processed properly or exposed to high humidity/temperature conditions. There were recalls of the tacrolimus ASD products due to their failure to meet critical quality attributes. The clinical performance of ASD can only be ensured if the amorphous/crystalline ratio meet its release specification and maintain that ratio/fraction throughout product shelf life. We have identified recall of tacrolimus drug product. It is due to crystallization of the amorphous drug that may results in clinical failure. We also developed analytical methods to quantify crystalline fraction in the drug

product. These methods were used by the industry for approval of generic and brand products of tacrolimus. We have published five papers on various quality aspects of tacrolimus.[74-75]

Theophylline has a narrow therapeutic index, with 12–25% of overdose patients developing serious or life-threatening symptoms. Age >60 years and chronic use are risk factors for increased morbidity and mortality. In acute overdose, peak serum levels >100 μg ml^{-1} may be predictive of arrhythmias and seizures. It is commercially available as immediate and extended release formulations. Understanding the impact of pharmaceutical processing, formulation excipients and their interactions on the solid-state transitions of pharmaceutical solids during use and in storage is critical in ensuring consistent product performance. We reported for first time effect of polymer viscosity, diluent type, granulation, and granulating fluid (water and isopropanol) on the pseudopolymorphic transition of theophylline anhydrous (THA) in controlled release formulations as well as the implications of this transition on critical quality attributes of the tablets. Although all freshly prepared formulations contained THA, the hydration-dehydration process induced during aqueous wet granulation hastened the pseudopolymorphic conversion of theophylline during storage through a cascade of events. On the other hand, no solid-state transformation was observed in directly compressed formulations and formulations in which isopropanol was employed as a granulating fluid even after the twelve weeks study period. The transition of THA to TMO resulted in a decrease in dissolution while an increase in dissolution was observed in directly compressed and IPA granulated formulation. Consequently, the impact of pseudopolymorphic transition of theophylline on dissolution in controlled release formulations may be the net result of two opposing factors: swelling and softening of the tablets which tend to favor an increase in drug dissolution and hydration of theophylline which decreases the drug dissolution. We have published our findings in *Journal of Pharmaceutical Sciences* and *International Journal of Pharmaceutics*.[79-80]

One of reasons for formulating drugs into modified release is to improve patient compliance. Other reasons are to improve safety, efficacy, and consistency in clinical outcome of drugs. Most commonly used extended release dosage forms are tablets and capsules. Modified release formulations include extended, sustained, controlled, and delayed release. The modified release formulations could be matrix tablets/capsules or film coated tablets/capsules containing film coated minitablets/pellets. The drug release from modified release dosage forms is controlled by polymer matrix or insoluble film of the coating. An example of a polymer used as a matrix former for extended release formulations is hydroxypropyl methylcellulose (HPMC). Commercial extended release formulation based on HPMC matrix are Depakote ER (divalproex sodium) and Tegretol®-XR (carbamazepine). In functionally coated tablets/pellets, the insoluble film controls release of drugs e.g. cellulose acetate, ammonio methacrylate copolymer, ethyl cellulose, methacrylic acid copolymer, etc, I have published peer reviewed papers on sustained, extended release, abuse deterrent, delayed and osmotically controlled formulations in peer reviewed papers.[81-90]

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Measuring Bridge Frequencies by a Test Vehicle in Non-Moving and Moving States

by Yeong-Bin Yang, Member EUAS

Short Biography

Honorary Dean, School of Civil Engineering, Chongqing University, Chongqing 400045, China

Fengtay Chair Professor, Dept. of Construction Eng., National Yunlin Univ. of Science and Technology, Yunlin, Taiwan, 64002, R.O.C.

Professor Emeritus, Department of Civil Engineering, National Taiwan University, Taipei, Taiwan 10617, R.O.C.

Dr. Yeong-Bin Yang received his Ph.D. degree from Cornell University in 1984. He is a member of Chinese Academy of Engineering, foreign member of Austrian Academy of Sciences, and member of EU Academy of Sciences. Currently, he is Honorary Dean of Civil Engineering, Chongqing University, Feng Tay Chair Professor of National Yunlin University of Science and Technology (YunTech), and Professor Emeritus of National Taiwan University (NTU). Also, he is Editor-in-Chief of International Journal of Structural Stability and Dynamics, former President of Asian-Pacific Association of Computational Mechanics, and former Chairman of International Steering Committee of East Asia-Pacific Conference on Structural Engineering and Construction.

Previously, he was YunTech's President, Dean of College of Engineering, NTU, Chairman of Civil Engineering Department, NTU, and President of four societies in Taiwan: Institute of Engineering Education Taiwan, Chinese Institute of Civil and Hydraulic Engineering, Society of Theoretical and Applied Mechanics, and Chinese Society of Structural Engineering. He has published over 265 referred journal papers, focused on the following areas: structural nonlinear theory and analysis, vehicle-bridge interaction dynamics, train-induced wave propagation, and vehicle scanning method for bridges. In each area he has also published a monograph.

Measuring Bridge Frequencies by a Test Vehicle in Non-Moving and Moving States

Y.B. Yang, Hao Xu, Bin Zhang, Feng Xiong, Z.L. Wang

Eng. Struct., 2020, 203

Abstract

This paper presents the measurement results of bridge frequencies by a test vehicle in non-moving and moving states. The self-made test vehicle fitted with vibration sensors is a two-wheel trailer, intentionally used to simulate the theoretical single degree-of-freedom system. The two-span bridge selected is located in the Chongqing University campus. For the purpose of comparison, the bridge

frequencies were firstly measured by direct deployment of vibration sensors on the bridge. The dynamic properties of the test vehicle in the non-moving state, including the transmissibility, are examined in detail. Based on the measured car-body response, the contact-point response of the vehicle with the bridge was calculated by a backward procedure that allows the vehicle frequency to be eliminated. It was found that the vehicle in the non-moving state can catch more bridge frequencies than in the moving state. Both the car-body and contact-point responses agree well the results by direct measurement. But the contact-point response performs better than the car-body response, which can be used to detect the first few frequencies of the bridge, including the torsional frequency.

Invariant Isogeometric Formulations for Three-Dimensional Kirchhoff Rods

Y.B. Yang, Yazhou Liu, Y. T. Wu

Comp. Meth. Appl. Eng., 2020, 365.

Abstract

In the isogeometric formulation for three-dimensional Kirchhoff rods, the invariance is required such that rigid-body modes associated with translations and infinitesimal rotations can be exactly represented. By enforcing the invariance in the isogeometric formulation of the rod, the equilibrium of forces and moments at fixed ends is preserved, and the performance is improved considerably for elements of finite sizes. We recognize that not all existing isogeometric formulations are invariant for general geometry of rods. Though an alternative formulation based on the Frenet-Serret frame and rotation angle representation was shown to be invariant, it does not work for rods with vanishing curvature, while its accuracy is affected by the low continuity of the angle of twist used. Motivated by this, two new invariant isogeometric formulations are developed, through different interpolations for the angle of twist. One uses the derivatives of the NURBS functions as the basis for the angle-of-twist interpolation, and the other uses a mixed interpolation incorporating both the Lagrange and NURBS functions. Several representative numerical examples were prepared to verify the accuracy and robustness of the two new formulations. Particularly, for rods of variable curvatures simulated by elements of finite or large sizes, the proposed formulations are demonstrated to outperform the two existing ones mentioned in predicting the displacements, end reactions and stress resultants.

Energy Storage through Innovative Synthesis and Processing of Nanomaterials

by Leon L. Shaw, Member EUAS

Short Biography

Current Positions

- *Rowe Family Endowed Chair Professor in Sustainable Energy, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*
- *Professor of Materials Science and Engineering, Department of Mechanical, Materials & Aerospace Engineering, Illinois Institute of Technology (IIT), Chicago, Illinois, USA*

Education

Ph. D.	*Materials Science and Engineering, University of Florida, Gainesville, Florida, USA, 1992*
Minor	*Mechanics and Engineering Science, Univers. of Florida, Gainesville, Florida, USA, 1992*
M. S.	*Materials Science and Engineering, University of Florida, USA, 1992*
M. Eng.	*Mechanical Engineering, Fuzhou University, Fuzhou, Fujian, China, 1987*
B. S.	*Materials Engineering, Fuzhou University, Fuzhou, Fujian, China, 1980*

Professional Activities

Member Editorial Board for "Scientific Reports"
Member Editorial Board for "Batteries"
Member Editorial Board for "Journal of Sol-Gel Science and Technology"
Member International Advisory Committee of THERMEC' 2011, 2013, 2016, and 2018
Member ASM International
Member TMS
Member American Ceramic Society
Member Electrochemical Society
Guest Editor Metallurgical and Materials Transactions (1998), Materials Science and Engineering (1998,2001, 2007), Journal of Materials Engineering and Performance (2005), Journal of Materials Science (2011)

Awards and Honors

2020	*Fellow, International Association of Advanced Materials (IAAM)*
2020	*"Illinois Researchers to Know in 2020", Illinois Science & Technology Coalition (ISTC)*
2020	*"Excellence in Research Award for 2020", Department of Mechanical, Materials and Aerospace Engineering, Illinois Institute of Technology, Chicago, Illinois*
2019	*Member, EU Academy of Sciences (EUAS)*
2019	*Keynote Presentation on "Coating as a Potent Method to Enhance the Specific Capacity, Charge Rate and Cycle Life of Cathodes for Next-Generation Li-ion Batteries" at the 2nd International Conference on Materials Science and Materials Chemistry, London, United Kingdom*
2018	*Energy Award, International Association of Advanced Materials (IAAM)*
2018	*Energy Award Lecture on "Hierarchical Design and Synthesis of Si Anodes for Next-Generation Li-ion Batteries" in Plenary Session at* ***European Advanced Materials Congress (EAMC 2018),*** *Stockholm, Sweden*
2018	*Rave Award, Illinois Institute of Technology for outstanding student employment service*
2018	*First Place in the poster competition at the 2018 Joint Advanced Photon Source/Center for Nanoscale Materials (APS/CNM) Users Meeting, Argonne National Laboratory, USA*
2016	*Keynote Presentation on "Hierarchical Design and Synthesis of Nanomaterials to Enable High Capacity Rechargeable Battery Electrodes," at THERMEC'2016, Graz, Austria*
2015	*Key Scientific Article contributing to the Excellence in Energy Research, Renewable Energy Global Innovations*
2014	*Keynote Presentation on "High Voltage, High Capacity, Ambient Temperature Sodium-Based Flow Batteries" at Cleantech 2014, Washington DC, USA*
2013	*Keynote Presentation on "Energy Storage Enabled by Nanomaterials and Advanced Processing" at ISPlasma 2013, Nagoya, Japan*
2011	*NSF Highlights: "Next Generation Bone Implants: More Like the Real Thing"*
2011	*Outstanding Poster Award, MS&T' 2011, Columbus, OH, USA*

2010 The John & Virginia Towers Distinguished Lecture, Michigan Technological University
2006 Member, Connecticut Academy of Science and Engineering (CASE), Connecticut, USA
2006 "Highly Commended Paper for Excellence 2006", Emerald Group Publishing Limited
2006 Outstanding Faculty Member Award, the Materials Science and Engineering Program, University of Connecticut, Connecticut
2005 Fellow, World Academy of Materials and Manufacturing Engineering (AMME), Poland
2004 Fellow, ASM International
2003 Best Poster Award, the Solid Freeform Fabrication Annual Meeting, Austin, TX
2001 Outstanding Department Member Award, Department of Metallurgy and Materials Engineering, University of Connecticut, Connecticut
2000 Outstanding Junior Faculty Award, School of Engineering, University of Connecticut, Connecticut
1999 Outstanding Department Member Award, Department of Metallurgy and Materials Engineering, University of Connecticut, Connecticut
1999 Honorary Advisory Professorship, Harbin Institute of Technology, Harbin, China
1999 Honorary Guest Professorship, Fuzhou University, Fuzhou, China
1995 Olin Junior Faculty Development Award, Olin Corporation, Connecticut
1992 First Place of the ASM International Graduate Student Paper Contest, ASM International
1990 Lifetime Member of Alpha Sigma Mu (International Metallurgical Honorary Society)

Publications, Patents and Presentations

- *Over 300 publications (including 3 edited books, 12 book chapters, 210+ archival refereed journal articles, 4 editorial materials, and 77 conference proceedings)*
- *11,000 non-self citations with a h-index of 55 and an i10-index of 185 (Google Scholar)*
- *3 US patents granted and 4 US patents pending*
- *290+ presentations including more than 100 invited talks, keynote presentations and plenary lectures at various national and international conferences as well as a wide range of universities in and outside the United States.*

Leon Shaw's research fields and scientific interests are in the areas of nanomaterials synthesis, processing and microstructure control for energy storage and structural applications as well as additive manufacturing. In the last 10 years, Leon Shaw has focused on nanomaterials synthesis and processing for energy storage, particularly in the areas of hydrogen storage materials, Li-ion batteries, Na-ion batteries, and redox flow batteries. In the area of hydrogen storage materials, the focus is on synthesis and processing of nanostructured $LiNH_2$, Li_2NH, LiH, $LiBH_4$ and MgH_2 materials to achieve hydrogen release and uptake near room temperature with high gravimetric densities. Recent work on a new composite mixture of nano-$LiBH_4$ + nano-MgH_2 has resulted in reversible release and update of 5.0 wt.% H_2 at 265 ^oC. This reversible storage capacity is one of the highest capacities ever reported for the $LiBH_4$ + MgH_2 system at temperature $\leq$ 265 ^oC.

In the area of rechargeable batteries, research has been focused on synthesis and processing of nanostructured Si anodes, novel coatings on $Li(Ni_xMn_yCo_z)O_2$ cathodes, Li-S batteries, structural defect control of $NaCrO_2$ cathodes, and hybrid Na-based flow batteries. The most prominent advancement made in the area of rechargeable batteries is the design and synthesis of Si micro-reactor powder that exhibits unusual properties with ultrafast charging/discharging capability (10 to 15 min), high specific capacity (800 mAh/g), and long-lasting cycle life (1,000 cycles) simultaneously. Silicon micro-reactor powder is synthesized via a simple and industrially scalable method, which can pave the way for practical applications of Si micro-reactors in the future. The advancements made in the areas of rechargeable batteries and hydrogen storage materials have led to multiple keynote presentations, plenary lectures, and "Energy Award" in 2018 presented by International Association of Advanced Materials (IAAM) as well as news release by *DOE* Environmental Molecular Sciences Laboratory **(***EMSL), The Hydrogen Journal, Pacific*

Northwest National Laboratory (PNNL), the Battelle Newsletter, and *Renewable Energy Global Innovations.* Some key publications in these areas are as follows.

Recent Publications in Li-ion Batteries, Na-ion Batteries and Redox Flow Batteries

- Y. R. Prado, M.-T. F. Rodrigues, S. E. Trask, L. Shaw, and D. P. Abraham, "Electrochemical Dilatometry of Si-bearing Electrodes: Dimensional Changes and Experimental Design," *J. Electrochem. Soc*., 167, 160551 (2020).
- M. Luo, A. L. Ortiz, and L. Shaw, "Enhancing the Electrochemical Performance of $NaCrO_2$ through Structural Defect Control," *ACS Appl. Energy Mater*., 3 [7] 7216-7227 (2020).
- M. Ashuri, Q. He, and L. Shaw, "Improving Cycle Stability of Si Anode through Partially Carbonized Polydopamine Coating," *Journal of Electroanalytical Chemistry*, 876, 114738 (2020).
- J. Wei, L. Shaw and W. Chen, "First-Principles Prediction of Na Diffusivity in Doped $NaCrO_2$ Layered Cathode Materials with Van der Waals Interactions," *J. Phys. Chem. C*, 124, 12239 – 12248 (2020).
- M. Ashuri, Q. He, Y. Liu, and L. Shaw, "Investigation towards Scalable Processing of Silicon-Graphite Nanocomposite Anodes with Good Cycle Stability and Specific Capacity," *Nano Materials Science*, 2, 297-308 (2020).
- M. Luo, A. L. Ortiz, and L. Shaw, "Unraveling Processing-Structure-Electrical Conductivity Relationships of $NaCrO_2$ Cathodes for Na-ion Batteries," *J. Electrochem. Soc*., 166 (15) A3546-A3553 (2019).
- Chen, W. Yao, Q. He, M. Ashuri, J. Kaduk, Y. Liu, and L. Shaw, "Tunable $LiAlO_2/Al_2O_3$ Coating through a Wet-Chemical Method to Improve Cycle Stability of Nano-$LiCoO_2$," *ACS Applied Energy Materials*, 2, 3098-3113 (2019).
- K. Sahni, M. Ashuri, Q. He, R. Sahore, I. D. Bloom, Y. Liu, J. A. Kaduk and L. Shaw, "H_3PO_4 Treatment to Enhance the Electrochemical Properties of $Li(Ni_{1/3}Mn_{1/3}Co_{1/3})O_2$ and $Li(Ni_{0.5}Mn_{0.3}Co_{0.2})O_2$ Cathodes," *Electrochimica Acta*, 301, 8-22 (2019).
- L. Shaw and M. Ashuri, "Coatings – A Potent Method to Enhance Electrochemical Performance of $Li(Ni_xMn_yCo_z)O_2$ Cathodes for Li-ion Batteries," *Adv. Mater. Lett.*, 10 (6), 369-380 (2019).
- M. Ashuri, Q. He, Z. Shi, C. Chen, W. Yao, J. Kaduk, C. Segre, and L. Shaw, "Long-Term Cycle Behavior of Nano-$LiCoO_2$ and Its Post-Mortem Analysis," *Journal of Physical Chemistry C*, 123, 3299-3308 (2019).
- S. Emani, C. Liu, M. Ashuri, K. Sahni, J. Wu, W. Yang, K. Nemeth, and L. Shaw, "Li_3BN_2 as a transition metal free, high capacity cathode for Li-ion batteries," *ChemElectroChem*, 6, 320-325 (2019).
- Liu and L. Shaw, "A High Capacity, Room Temperature, Hybrid Flow Battery Consisting of Liquid Na-Cs Anode and Aqueous NaI Catholyte," *Batteries*, 4, 60 (2018).
- M. Ashuri, Q. He, Y. Liu, S. Emani, and L. Shaw, "Synthesis and Performance of Nanostructured Silicon/Graphite Composites with a Thin Carbon Shell and Engineered Voids," *Electrochimica Acta*, 258, 274-283 (2017).
- J. S. Shamie, C. Liu, L. Shaw, and V. L. Sprenkle, "New Mechanism for the Reduction of Vanadyl Acetylacetonate to Vanadium Acetylacetonate for Room Temperature Flow Batteries," *ChemSusChem*, 10 (3), 533-540 (2017).
- M. Sawicki, A. Ortiz, M. Luo and L. Shaw, "Structural-Defect-Controlled Electrochemical Performance of Sodium Ion Batteries with $NaCrO_2$ Cathodes," *ChemElectroChem*, 4, 3222-3230 (2017).
- L. Chen, N. L. Dietz Rago, I. D. Bloom, and L. Shaw, "New Insight into the Electrode Mechanism of Lithium Sulfur Batteries via Air-Free Post-Test Analysis," *Chem. Commun*., 52, 9913-9916 (2016).
- Liu, B. B. Koyyalamudi, L. Li, S. Emani, C. Wang, and L Shaw, "Improved Capacitive Energy Storage via Surface Functionalization of Activated Carbon as Cathodes for Lithium Ion Capacitors," *Carbon*, 109, 163-172 (2016).
- M. Ashuri, Q. He, Y. Liu, K. Zhang, S. Emani, M. S. Sawicki, J. S. Shamie and L. Shaw, "Hollow Silicon Nanospheres Encapsulated with a Thin Carbon Shell: An Electrochemical Study," *Electrochimica Acta*, 215, 126-141 (2016).
- M. Ashuri, Q. He and L. Shaw, "Silicon as Potential Anode Material for Li-ion Batteries: Where Size, Geometry and Structure Matter," *Nanoscale*, 8, 74-103 (2016).
- L. Chen, Y. Liu, N. Dietz-Rago and L. Shaw, "Bottom-up, Hard Template and Scalable Approaches toward Designing Nanostructured Li_2S for High Performance Lithium Sulfur Batteries," *Nanoscale*, **7, 18071-18080 (2015)**.
- C. Liu, J. S. Shamie, L. Shaw, and V. L. Sprenkle, "An Ambient Temperature Molten Sodium-Vanadium Battery with Aqueous Flowing Catholyte," *ACS Appl. Mater. Interfaces*, 8, 1545-1552 (2015).
- L. Chen, Y. Liu, F. Zhang, C. Liu and L. Shaw, "PVP-Assisted Synthesis of Uniform Carbon-Coated Li_2S/CB for High Performance Lithium Sulfur Batteries," *ACS Appl. Mater. Interfaces*, 7, 25748-25766 (**2015).**
- M. Sawicki and L. Shaw, "Advances and Challenges of Sodium Ion Batteries as Post Lithium Ion Batteries," RSC Advances, 5, 53129-53154 (2015).
- J. S. Shamie, C. Liu, L. Shaw, and V. L. Sprenkle, "Room Temperature, Hybrid Sodium-Based Flow Batteries with Multi-Electron Transfer Redox Reactions," *Scientific Reports*, 5, 11215 (2015).
- C. Wang, M. Sawicki, S. Emani, C. Liu, and L. Shaw, "$Na_3MnCO_3PO_4$ – A High Capacity, Multi-Electron Transfer Redox Cathode Material for Sodium Ion Batteries," *Electrochimica Acta*, 161, 322-328 (2015).
- L. Chen, Y. Liu, M. Ashuri, C. Liu and L. Shaw, "Li_2S Encapsulated by Nitrogen-Doped Carbon for Lithium Sulfur Batteries," *J. Mater. Chem. A*, **2 (42), 18026 – 18032 (2014)**.
- L. Chen and L. Shaw, "Recent Advances in Lithium-Sulfur Batteries," *J. Power Sources*, 267, 770 – 783 (2014).

Recent Publications in Hydrogen Storage Materials

- Z. Ding, H. Li, and L. Shaw, "New Insights into the Solid-State Hydrogen Storage of Nanostructured $LiBH_4$-MgH_2 System," *Chemical Engineering Journal*, 385, 123856 (2020).
- G. Yan, H. Li, Z. Ding, W. Yang, Z. Gao, W. Ma, and L. Shaw, "Mechanism of Hydrogen Storage on Fe_3B," *Chem. Commun*., 56, 14235 (2020).
- Z. Ding, Z. Chen, T. Ma, C.-T. Lu, and L. Shaw, "Predicting the Hydrogen Release Ability of $LiBH_4$-based Mixtures by Ensemble Machine Learning," *Energy Storage Materials*, 27, 466 – 477 (2020).
- Z. Ding, S. Li, Y. Zhou, Z. Chen, W. Ma, and L. Shaw, "$LiBH_4$ for Hydrogen Storage: New Perspectives," *Nano Materials Science*, 2 [2] 109 – 119 (2020).
- Z. Ding, Y. Lu, L. Li, and L. Shaw, "High Reversible Capacity Hydrogen Storage through Nano-$LiBH_4$ + Nano-MgH_2 System," *Energy Storage Materials*, 20, 24-35 (2019).
- Z. Ding, P. Wu, and L. Shaw, "Solid-state hydrogen desorption of $2MgH_2$ + $LiBH_4$ nano-mixture: A kinetics mechanism study," *J. Alloys Compd.*, 806, 350 – 360 (2019).
- Z. Ding and L. Shaw, "Enhancement of Hydrogen Desorption from Nanocomposite Prepared by Ball Milling MgH_2 with in situ Aerosol Spraying $LiBH_4$," *ACS Sustainable Chem. Eng.*, 7 (17), 15064-15072 (2019).
- Y. Zhong, X. Wan, Z. Ding and L. Shaw, "New dehydrogenation pathway of $LiBH_4$ + MgH_2 mixtures enabled by nanoscale $LiBH_4$," *Int. J. Hydrogen Energy*, 41, 22104-22117 (2016).
- Z. Ding, X. Zhao, and L. Shaw, "Reaction between $LiBH_4$ and MgH_2 induced by high-energy ball milling," J. Power Sources, 293, 236-245 (2015).

Novel nanomaterial synthesis and processing are expected to continuously lead to advanced materials with new functionalities and superior properties. In particular, microstructure control and crystal defect manipulation made available by novel nanomaterial synthesis and processing have the potential to result in new materials with unprecedented properties for energy storage and structural applications in the future.

Recent Developments on Sustainable Urban Infrastructure Systems

by John C. Crittenden, Member EUAS

Short Biography

Director of the Brook Byers Institute for Sustainable Systems
Hightower Chair and GRA Eminent Scholar in Sustainable Technologies
School of Civil and Environmental Engineering – Georgia Institute of Technology

EDUCATION

University of Michigan, Ann Arbor:	*B.S. Chemical Engineering*	*1971*
University of Michigan, Ann Arbor:	*M.S. Civil and Environmental Engineering*	*1972*
University of Michigan, Ann Arbor:	*Ph.D. Civil and Environmental Engineering*	*1976*

HONORS: *National, international, state, and regional awards for research and teaching excellence.*

These are sample awards:

2020 Simon W. Freese Environmental Engineering Award and Lecture, American Society of Civil Engineers (ASCE)
2020 Future of Photocatalysis Paper Winning Best Feature Paper Award, American Chemical Society
2019 Chinese Government Friendship Award
2016 Elected as a Fellow of the American Society of Civil Engineers
2015 Chinese Academy of Sciences President's Distinguished Scientist Award
2015 Athalie Richardson Irvine Clarke Prize, National Water Research Institute
2014 Alumni Merit Award, University of Michigan, Department of Civil and Environmental Engineering
2013 Elected to the Chinese Academy of Engineering
2008 Recognized by the American Institute of Chemical Engineers as one of the "100 Chemical Engineers of Modern Era" in the category of "New Frontiers"
2002 Elected to the National Academy of Engineering
2000 AEESP Landmark Achievement Award presented annually to authors
1991 Recipient of the Walter L. Hubert Research Prize, awarded by ASCE for Research Contributions on Removal of Organics from Water
1989 Corecipient of the American Water Works Association Publication's Award for the paper which represents the most significant advancement in science and engineering as it applies to water supply practices
1980 Corecipient of the Rudolph Hering Medal awarded by ASCE for the most valuable contribution to the Journal of Environmental Engineering Division Proceedings of ASCE

RESEARCH EXPERIENCE: *Sustainability, Pollution Prevention, Physical-Chemical Treatment Processes (Ion Exchange, Oxidation Processes, Catalytic Oxidation, Photocatalytic Oxidation, Electro-catalysis, Adsorption, Electro-Adsorption, Air Stripping), Transport of Organics in*

Saturated and Unsaturated Groundwater, Modeling of Fixed-Bed Reactors and Adsorbers (Photocatalysis, Low Temperature Catalysis in Aqueous and Gas Phases, Transport of Organics in Saturated and Unsaturated Groundwater), Sol-Gel Chemistry for Preparation of Zeolites and Catalysts, Surface Chemistry and Thermodynamics (Prediction of Adsorption Capacities and Surface Catalyzed Rate Constants), Mass Transfer, Numerical Methods, Modeling of Wastewater and Water Treatment Processes

PROFESSIONAL EXPERIENCE: *Georgia Institute of Technology 2009-present. Arizona State University 2004-08. Michigan Technological University 1979-2003. University of Illinois 1978-1979. Washington State University 1977-1979. Consultant to over 45 utilities, companies and universities worldwide on adsorption technology, water quality modeling, advanced oxidation, pollution prevention since 1975.*

COURSES TAUGHT*: Sustainable Engineering, Water Chemistry, Physical and Chemical Treatment of Air and Water, Reactor Engineering, Separation Technologies and Unit Operations in Environmental Engineering, Hydromechanics, Water and Wastewater Treatment, Intro to Environmental Engineering*

RESEARCH PROJECTS: *Seventy-two research projects were successfully completed in the last 40 years. These grants and contracts accounted for $56 million in funding in the areas of sustainable infrastructure, pollution prevention, air stripping, advanced oxidation, adsorption, and groundwater transport.*

PUBLICATIONS: *403 publications in refereed journals, 15 books and chapters, and 161 reports or contributions to proceedings. Six copyrighted software products and seven patents in the areas of pollution prevention, stripping, advanced oxidation/catalysis, adsorption and groundwater transport. These are some sample publications:*

Prof. John C. Crittenden is the director of the Brook Byers Institute for Sustainable Systems and a professor in the School of Civil and Environmental Engineering at the Georgia Institute of Technology. He holds the Hightower Chair and is a Georgia Research Alliance Eminent Scholar in Environmental Technologies. Prof. Crittenden received his Bachelor's in Chemical Engineering and his Master's and Ph.D. in Civil Engineering from the University of Michigan. Prof. Crittenden was elected to the US National Academy of Engineering in 2002 and the Chinese Academy of Engineering in 2013. He is the 2015 Clarke Prize laureate, which is generally recognized as the American Nobel prize for water and received the 2020 Simon W. Freese Environmental Engineering Award and Lecture for his extraordinary accomplishments in using fundamental scientific principles and current research findings to solve the most challenging water quality problems (American Society of Civil Engineers. He is the co-holder of five patents and the primary author of the bestselling textbook, Water Treatment: Principles and Design, now in its third printing (2012, Wiley). He is the author more than 372 articles that were published in refereed journals, more than 100 book chapters, reports, and symposia and has more than 30,000 citations and a H index of 75.

Prof. Crittenden's current research focus is on sustainable urban infrastructure systems. His colleagues and he are conducting research on alternative energy technologies, sustainable materials, food energy water nexus, advanced modeling of urban systems, sustainable engineering pedagogy, and urban form and policy. He also conducts research in various water and air treatment technologies (e.g.,

membrane technology, advanced oxidation processes, photocatalytic oxidation, adsorption, selective catalytic reduction) and energy harvesting technologies (photocatalytic water splitting and aqueous phase reforming of biomass).

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Energy Sustainability

by Marc A. Rosen, Member EUAS

Short Biography

Education

- *Ph.D., 1987, Univ. of Toronto, Dept. of Mechanical Engineering*
- *M.A.Sc., 1983, Univ. of Toronto, Dept. of Mechanical Engineering*
- *B.A.Sc., 1981, Univ. of Toronto, Div. of Engineering Science, Nuclear and Thermal Power Generation Option*

Recent Professional Experience

- *Professor, Faculty of Engineering and Applied Science, Univ. of Ontario Institute of Technology, Oshawa, Ontario, 2002-pres.*
- *Dean (founding), Faculty of Engineering and Applied Science, Univ. of Ontario Institute of Technology, Oshawa, Ontario, 2002-08.*
- *Chair, Dept. of Mechanical Engineering, Ryerson Polytechnic Univ., Toronto, 1994-99.*
- *Director, School of Aerospace Engineering, Dept. of Mechanical Engineering, Ryerson Polytechnic Univ., Toronto, 1992-94.*

Other Significant Professional Positions

- *Editor, Energy Conversion and Management, 2013-pres.*
- *Editor-in-Chief, Int. Journal of Energy and Environmental Engineering, 2012-pres.*
- *Editor-in-Chief, Sustainability, 2009-pres.*
- *Editor-in-Chief, Biofuels, 2014-pres.*
- *President, Engineering Institute of Canada, 2008-10.*
- *Director, Durham Strategic Energy Alliance, 2005-07.*
- *President, Canadian Society for Mechanical Engineering, 2002-04.*

Honours and Awards

- *John B. Stirling Medal, Engineering Institute of Canada*
- *Educational Award of Honour, Minerva Canada*
- *President's Award, Canadian Society for Mechanical Engineering*
- *Engineering Alumni Hall of Distinction, University of Toronto*
- *Andrew H. Wilson History Award, Canadian Society for Mechanical Engineering*
- *C.N. Downing Award, Canadian Society for Mechanical Engineering*
- *Julian C. Smith Medal, Engineering Institute of Canada*
- *Robert W. Angus Medal, Canadian Society for Mechanical Engineering*
- *Fellow, American Society of Mechanical Engineers*
- *Fellow, Engineering Institute of Canada,*
- *Fellow, International Energy Foundation*
- *Fellow, Canadian Society for Mechanical Engineering*
- *Fellow, Canadian Society for Senior Engineers*

Principal Areas of Interest

- *Thermodynamics: Second-Law Analysis. Theoretical development; use in simulation codes; application to improve efficiency and performance of engineering systems.*
- *Energy Sustainability and Energy Systems Analysis. Analysis, design, modelling, simulation and optimization; environmental assessment; energy-environment ties.*
- *Energy Technologies. District energy, thermal energy storage, solar energy, hydrogen energy, nuclear energy, electricity generation and cogeneration, chillers, synthetic fuels production, integrated energy systems.*
- *Heat Transfer. Modelling, simulation and analysis computationally and analytically.*

Achievements Related to Energy Sustainability

Dr. Marc A. Rosen has over his entire career been active in the area of energy, including efficiency, environmental impact and sustainability. He also has taken on key leadership roles for institutions in transformation throughout his career. Many of these achievements have directly and indirectly supported energy sustainability, its applications, and developments of related journals and engineering societies.

As Founding Editor-in-Chief of the journal *Sustainability*, published by MDPI, Dr. Rosen led the journal's development and growth from its launch in 2009 to the point where it now is a leading venue for the publication of research and application articles related to sustainability and sustainable development. The journal is an international, cross-disciplinary, scholarly and open publication for environmental, cultural, economic, and social sustainability of humanity. It now has 21 sections and over 10,500 publications annually. This journal has proven transformative in helping advance the field of sustainability while having a global extent and impact. Dr. Rosen also has been heavily involved in the lead conference sponsored by that journal, the World Sustainability Forum. He was the general chair of the first four World Sustainability Forums, and has been heavily involved in subsequent Forums, often delivering keynote presentations.

As Founding Dean of Engineering and Applied Science at Ontario Tech University (University of Ontario Institute of Technology), Dr. Rosen launched an new engineering school, premised on innovative approaches to teaching and learning and on market-oriented research. He also helped build Ontario's first new university in 40 years, one with engineering and technology as its primary area and with energy as one key research and educational focus, and sustainable energy as a theme in much of that activity. There is a strong focus on energy and energy sustainability in many graduate and undergraduate programs that Dr. Rosen helped create. In response to the need for better business and management skills in engineering, Dr. Rosen launched for each engineering program an innovative Engineering and Management version.

Dr. Rosen was instrumental in attaining for his university an institution-defining $100 million Automotive Centre of Excellence, in collaboration with industry, an institution-defining achievement since Ontario Tech's creation in 2002. The Automotive Centre of Excellence is supportive for the development and testing of future vehicles, including sustainable vehicles (e.g., vehicles that operate on alternative fuels like hydrogen, and electric vehicles).

Prior to joining Ontario Tech University, Dr. Rosen was a professor in the Department of Mechanical, Aerospace and Industrial Engineering at Ryerson University. During his tenure at Ryerson, Dr. Rosen served as department Chair, and Director of the School of Aerospace Engineering. He played a key role in launching graduate programs, expanding research, obtaining accreditation for engineering programs. Dr. Rosen also was a lead developer and player in the university's multidisciplinary program in Environmental Science and Management and he led the creation of thermofluids and energy options within Mechanical Engineering at the undergraduate and graduate levels, and helped ensure sustainability concepts and applications pervade throughout, via such avenues as advanced training in renewable energy sources.

Lately, his teaching of sustainability, and indeed much of his research and other activity, has incorporated and been guided by the new United Nations Sustainable Development Goals.

With over 70 research grants, Dr. Rosen is an active industry collaborator, with much of his research adopted by industry. His innovations have led to increased sustainability and

efficiency in energy technologies, improved alternative technologies (like solar, hydrogen and storage technologies), and reduced environmental impact. He was a key player in a two projects (valued at over $10 million) to produce hydrogen from nuclear energy and other renewable thermal forms of energy, in industrial quantities. He was co-Principal Investigator of the second of these projects. He also was a theme leader in a $12 million project on net-zero energy buildings, which has advanced the development of buildings that use, on average, zero energy over the year. Implementing such technology can reduce Canada's energy use and environmental emissions by up to 30%. His noteworthy engineering accomplishments include advancing energy systems to make them more sustainable and less environmentally damaging through innovative research, and collaborating with industry to facilitate the adoption of those innovations.

Some notable examples of Dr. Rosen's research and its impact follow. His research has led to sustainable energy systems, buildings and communities [1-3], and to improvements in the sustainability of transportation technologies of various kinds, especially automobiles, trains and aircraft [4]. Some of his research has led to improvements in the sustainability of manufacturing, production and economic systems. [5-6]. Dr. Rosen's research has also focused on the large scale, including an assessment of the sustainability national energy systems like Canada's [7].

Dr. Rosen has published almost 700 journal articles in leading journals, a large fraction addressing sustainability, and authored or co-authored over 110 book chapters as well as 21 books, many directly linked to sustainability [8-12]. These books include the ground-breaking work by Dr. Rosen on the linkages between the thermodynamic quantity "exergy" and sustainability, extending beyond thermodynamics to environment, ecology and economics, challenging convention and leading to new understandings of sustainability. His books on thermal energy storage, exergy, exergy and the environment, and exergy and economics are considered by many to be seminal. In addition, Dr. Rosen has authored or co-authored many books that deal indirectly with sustainability, by focusing on technologies that facilitate energy sustainability [13-17]. Dr. Rosen has also published extensively on engineering ethics and safety.

As a Director of Oshawa Power for over a decade, a local electrical distribution company that serves a city of about 160,000 people, Dr. Rosen helped that utility's expansion into sustainable energy forms and technologies like solar photovoltaics, wind, and biomass and cogeneration.

During his tenure as President of the Engineering Institute of Canada, Dr. Rosen assisted in affirming its leadership role and helped in developing a vision statement for EIC that had sustainability at its core, being phrased "Engineering for a prosperous, safe and sustainable Canada." The Engineering Institute of Canada was founded in 1887 and is a federation of leading Canadian engineering societies. Dr. Rosen also helped revitalize the Canadian Society for Mechanical Engineering during his term as President. He chaired that society's Technical Division on Thermofluids Engineering for two decades, focusing on advancements in renewable energy technology and sustainable energy. He has served the Canadian Engineering Accreditation Board (CEAB), and chaired the Judging Committee the Canadian Consulting Engineering Awards. He is editor-in-chief of several noteworthy international journals, devoted to topics like sustainability, energy and the environment.

Dr. Rosen has been extensively involved in international activities, including the development and implementation of a joint distance education course in Pollution Prevention in Brazil, with the support of the Canadian International Development Agency. This project led to a book. He was also his Department's lead contact for five years in the North American Design Institute (NADI), which facilitate exchanges between Mexico, the

U.S. and Canada. In addition, Dr. Rosen served on several industrial and academic advisory committees, including Canadian Representative on the International Energy Agency (IEA) Experts Group on Cogeneration/District Cooling.

Impact and Significance on Energy Sustainability

The significance of Dr. Rosen's achievements are described in more detail below. They have been in four main areas: advancement of industry, research, education and the engineering profession, and have had a significant impact on each. All of these achievements have helped in the development and application of sustainability and especially energy sustainability.

Much of Dr. Rosen's research has been adopted by industry, and helped to improve energy use, mitigate environmental impact, and increase efficiency. He has written over 50 technical reports that attest to this. One project identified efficiency improvements in power plants at Ontario Power Generation. Another project provided compelling evidence of the benefits of cogeneration, convincing large electrical power utilities to implement cogeneration. A third project aims to have Canada's nuclear reactors produce hydrogen for transportation, industry and supporting the oil sands development. Industry benefits resulted from his service as the Canadian Representative on the International Energy Agency Experts Group on Cogeneration/District Cooling. Finally, another aims at reducing the energy use for Canada's building stock, presently responsible for a third of the nation's energy use, to zero. The economic value of the projects he has been involved with directly as a principal or co-investigator exceeds $30 million.

Dr. Rosen has also carried out work directly on or related to sustainability for a range of national and international companies, such as Imperial Oil Ltd., General Electric, Bell Canada, Apotex Inc., FuelMaker Corporation, and Inst. for Hydrogen Systems. As well, he has carried out projects for various government agencies at the international, national and provincial levels, including International Energy Agency, Natural Resources Canada, Environment Canada, Ontario Ministry of the Environment, and Ontario Ministry of Community and Social Services.

Dr. Rosen has advanced thermodynamic methods, cogeneration, district energy, thermal storage, renewable energy, and environmental stewardship. One of the most significant achievements of Dr. Rosen has been his work to advance the methodology and framework for holistic assessments of sustainability. This has been carried out by Dr. Rosen for engineering activity in general, and for energy-related work in particular [18-20]. Applications of the above work are numerous and include an assessment of the contributions to regional sustainability of the Dead Sea-Red Sea project involving Israel, Jordan and the Palestinian Authority [21]. His work has also led to advanced optimization methods, with applications in various fields [22].

Dr. Rosen has advanced engineering education, through his many roles in universities. In particular, he helped create a new research intensive university focused on technology. In leading the launch of the Faculty of Engineering and Applied Science at Ontario Tech University, Dr. Rosen created the vision of a new engineering school which would be premised on the use of innovative educational methods and technologies, and value-added research that is closely tied to the marketplace and contributes to society. His university's Faculty of Engineering and Applied Science uses a laptop computer and webcentric learning approach. On the teaching front, Dr. Rosen has been innovative, creating several new courses at the graduate and undergraduate levels. Two examples are graduate courses

on Energy and the Environment and Pollution Prevention. In addition, Dr. Rosen helped develop a Faculty-wide course on law, ethics and professionalism for engineers. During his years in academe, he has also developed innovative options and streams in programs. Sustainability features in all of these courses.

He has also been involved in the American Society of Heating, Refrigerating and Air-Conditioning Engineers on sustainability, by serving as corresponding member for a technical group on exergy analysis for sustainable buildings. As a member of the Advisory Committee for Sustainable Energy Solutions for the Ontario Centres of Excellence, Dr. Rosen helped advance the sustainability of various earth and environmental technologies. As a director of the Durham Strategic Energy Alliance, Dr. Rosen helped lead development of a regional energy focus in Durham, to help address Ontario's and Canada's energy challenges. Finally, as a review committee member on the International Thermonuclear Experimental Reactor, Dr. Rosen advised the Canadian and Ontario governments on the prospects and benefits of fusion energy.

Dr. Rosen has been extensively recognized for his achievements in engineering, education and research, and distinguished service to learned societies. He has received best paper awards (e.g., "Energy and Exergy Analyses of Power Generation via an Integrated Biomass Post-Firing Combined-Cycle" at an IEEE International Conference on Smart Energy Grid Engineering). Dr. Rosen is a fellow of the Canadian Society for Senior Engineers, the Canadian Academy of Engineering, the American Society of Mechanical Engineers, the Engineering Institute of Canada, the International Energy Foundation and the Canadian Society for Mechanical Engineering. He was elected to University of Toronto's Engineering Alumni Hall of Distinction.

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The Process of Consciousness and Its Evolution Arising from Granulation and Bilogic

by Fionn Murtagh, Member EUAS

Short Biography

Degrees listed backwards in time, and very initial work in companies.

1993, HDR (Habilitation à diriger des recherches), "Méthodes de reconnaissance des formes en astronomie" ("Pattern Recognition Methods in Astronomy"), Université de Strasbourg.

1981, PhD – Doctorat de 3ème cycle (Mathematical Statistics), "Classification et discrimination sous contrainte de contiguîté continue" ("Classification and discrimination subject to a continuous contiguity constraint"), Université P&M Curie, Paris 6, in collaboration with BRGM, Bureau de Recherches Géologiques et Minières, Orléans.

1979, MSc (Computer Science – Information Retrieval), Trinity College Dublin.

1976, BA (Mathematics), BAI (Engineering Science), Trinity College Dublin.

1972, Leaving Certificate (O'Connell's School, Dublin). Institute of Physics medal for First place in Ireland in Physics.

In secondary school, this included some months each summer in the national train engineering and production centre in Dublin, including a wide range of production and maintenance; in the Guinness brewery, in the Cadbury chocolate and food factory, in Dublin, and in Brown Boveri & Cie., in Baden, Switzerland, which later merged with Asea to become ABB, Asea Brown Boveri.

Work listing backwards in time.

Following retirement in July 2020, to be Professor Emeritus.

1 June 2017 to now, Professor of Data Science, University of Huddersfield,
Director of a Centre that is to become an Institute of Mathematics and Data Science, Courses include
new BSc in Mathematics, MSc in Data Analytics, and soon an MSc in Industrial Mathematics.
I was External Examiner in the Ulster University, Northern Ireland, for a few years, and I am still now, External Examiner for Mathematics, Master and undergraduate degrees in University of Essex. BICDaS (Bielefeld Center for Data Science) Advisory Board Member, Bielefeld, Germany.

May 2015 to end of May 2017, Professor of Data Science, University of Derby (not one day per week), and for about two years, one day per week, Professor of Data Science, Goldsmiths, University of London. My MSc course, in the MSc of Data Science, it was "Geometric Data Analysis", i.e. Correspondence Analysis, I am continuing to be Visiting Professor in Goldsmiths.

July 2013 to end of 2014, Professor and Head of School, School of Computer Science and Informatics, De Montfort University, Leicester.

2004 to 2013, Professor of Computer Science, Royal Holloway University of London (RHUL), and 2005-2007, Head of Department of Computer Science. For RHUL, I am now Honorary Professor in Computer Science and also Fellow, Computer Learning Research Centre. (The following was with leave of absence from RHUL.)

October 2007 to October 2012, Director, Information Communications and Emergent Technologies, Science Foundation Ireland (SFI), Dublin .(For funding of research proposals, there was a lot of contact with Government Ministers, and with University Presidents.)

1988 to 2007, Professeur Associé Sciences et Techniques (Adjunct Professor) Astronomical Observatory,

University of Strasbourg, France.
1999-2004, Professor of Computer Science, Queen's University Belfast (Northern Ireland). (Executive Member of the Medical Imaging Forum of Northern Ireland.)
1996-1999, Professor of Computing, Magee Campus, Derry (Northern Ireland), University of Ulster (now) Ulster University. There I set up my company, Multi Resolutions Ltd.
1984-1996, Senior Scientist, Space Science Department, European Space Agency.
Based at the European Southern Observatory (ESO), Garching/Munich, on the Hubble Space Telescope (HST) project. (By the summer of 1993, I set up and managed ESO's web site on two continents, Europe and South America.) (The web as we know it effectively started in 1993.)
(When Neural Networks were developed, we had a day giving presentations with a company in Munich.) For Hubble Space Telescope, there were many meetings in the United States.
1984, Scientist, Joint Research Centre, Ispra, northern Italy.
1980-1984, Lecturer, Computer Science, University College Dublin (UCD). (Head of Department was Professor Keith van Rijsbergen). (I will be Visiting Professor in UCD.)
1976-1978 (one year full-time, and then one year half time, because I was doing my MSc), Statistician-Programmer, Educational Research Centre, St Patrick's College, Dublin. (St. Patrick's College, developing school teachers, is now in DCU, Dublin City University).
Award, Medal and Certificate
Outstanding Contributions to Astrostatistics Award 2016. Awarded, May 2016, by: IAA Awards, International Astrostatistics Association. See: http://www.cambridge.org/us/academic/international-astrostatistics-association-award-winners. Commendation: "For his long time contributions to astroinformatics and related areas in the computational sciences; advancing scientific knowledge in classification theory and image analysis; for his contributions to the success of the Hubble Space Telescope; for his role on the organizing committee of the IAU Commission B3 on Astroinformatics Astrostatistics; and for his long time efforts in dealing with the statistical analysis of "Big Data".

The Process of Consciousness and Its Evolution Arising from Granulation and Bilogic

Abstract

Our objective is to seek symmetry originating in the unconscious, and that is expressed here as reporting in consciousness. The association of psychological constructs that are consciousness and unconscious are to be both understood and interpreted within Ignacio Matte-Blanco's theory and his Bilogic framework. We carry out text mining, using extensively recorded dream reports. The texts themselves, and all the content, termed word corpus, are mapped into real-valued semantic, factor space, using Correspondence Analysis that can also be termed Geometric Data Analysis. Factors can be interpreted. For granulation, this new development is carried out: for texts and words, their factor projections are ternary encoded, to express commonality and exceptionalism. Then determined are clusters of terms and of words with semantic identity. Hence an innovative approach to granulation, and mostly with linear computational complexity. The study here establishes new implementation in analytical methods, and is also to have definite reproducibility in other, relevant and associated domains.

This work can be pursued in other application domains, to have processing and evolution analyzed in surveys, and in social science.

This book of mine, Murtagh, F. (2017), **" Data Science Foundations: Geometry and Topology of Complex Hierarchic Systems and Big Data Analytics"**. Chapman and Hall/CRC, Boca Raton, Florida,

One emphasis is that Data Science can and should have full relationshop between

methodology and domain (or domains) of application. Correspondence Analysis, also termed in some other books, Geometric Data Analysis, it maps qualitative data into factor space, with Euclidean metric, and common clustering is hierarchic clustering.

A number of new books are being planned to be later published, one is for Data Science and Criminology, another is Data Science and Artificial Intelligence in Healthcare, and another perhaps is for the mathematics of the early development of the Universe.

Google Scholar has me with h-index 63 and some of my colleagues and collaborators have h-index of 104 and 118. For me, there are 19,783 citations of my publications.
So far, the number of my books that are authored or also edited, there are 29 books; for Journal papers, there are 177; then contributed articles: 42; and in conference proceedings and in edited volumes: there are 139.

There are many other both publications and plans – the latter includes planning for projects.

F. Murtagh and K. Devlin, **"The Development of Data for Sustainable Development", Big Data and Cognitive Computing**, 2(2), 14, 2018.
Access: https://www.mdpi.com/2504-2289/2/2/14

In this paper there is a reference to how some European project proposals have more than 98% unaccepted:
F. Murtagh, M. Orlov and B. Mirkin, "Qualitative Judgement of Research Impact: Domain Taxonomy as a Fundamental Framework for Judgement of the Quality of Research", **Journal of Classification**, 35(1), 5-28, 2018.
Preprint prior to submission: https://link.springer.com/article/10.1007/s00357-018-9247-0
Books and papers are listed on this web site (then with at the end of this web address:pubs)
http://www.multiresolutions.com/home/

On that web site, I hope to have all journals listed where I am on the Editorial Board. For the Computer Journal, I had been Editor-in-Chief for about ten years of the Computer Journal, the British Computer Society's flagship journal. Now I am section editor for Section C: Computational Intelligence, Machine Learning and Data Analytics. In general there are always 172 submissions for Section C, and I ask Editorial Board members to be Handling Editors, and I have about 32 papers myself as Handling Editor. A very large number of submissions, are from researchers in India and China. Now more in total than 1000 per year.

Each year, I do other reviewing, for journals when I have the time to do it, and in the past book proposals, and also sometimes each year research funding proposals for various countries, in Europe, Russia, Canada.

I have a leading role in classification societies: I am ex-President of the Classification Society of North America, now titled Classification Society, and a Board Member for many decades, and again now President of the British Classification Society, a Council Member of International Statistical Institute (ISI), as well as long term member, and Fellow of the British Computer Society, and a Fellow of many other organisations. For ISI,

the World Statistics Congress (in 2019 in Malaysia, in 2017 in Morocco, to be in 2023 in Canada, in July 2021, in the Netherlands, and to be online because of the Covid-19 pandemic. I am a Board Member of EuADS, European Association of Data Science. We are to have a Summer School of EuADS in July 2021, and I have to have one course in it.

I am an elected member of the scholarly academies, the Royal Irish Academy and Academia Europaea, and, here, EUAS, EU Academy of Sciences. I have been awarded Fellowships in many organisations, including: Institute of Mathematics and Its Applications (IMA), Royal Statistical Society. Also of course, ACM and IEEE. I have stated to have been a lead investigator in winning about £60 million in research funding. (But in 2020, I was associated with a European proposal, led by an institute in Germany, it was for Artificial Intelligence in Medical work, but it did not get accepted; some time ago there were three times the submission of a European project, IoT, Internet of Things, for elderly people in houses, but that did not get accepted for the three years it was submitted, and another project, submitted two times, led by a colleague in France, that did not get accepted in the two years it was submitted.)

Discovery of Regucalcin: Genomics, Cell Regulation and Diseases

by Masayoshi Yamaguchi, Member EUAS

Short Biography

Masayoshi Yamaguchi, Ph.D., IOM, FAOE, DDG, DG, is Full Professor, University of Hawaii Cancer Center, University of Hawaii at Manoa, Honolulu, USA (2020-); Adjunct Professor, University of Hawaii Cancer Center, University of Hawaii at Manoa (2019-); Visiting Professor, David Geffen School of Medicine, University of California, Los Angeles (UCLA) (2017-2019); Adjunct Professor, Emory University School of Medicine, Atlanta,, USA (2013~2016); Visiting Professor in Department of Medicine, Baylor College of Medicine, Houston, USA (2012–2013); Visiting Professor, Department of Medicine, Emory University School of Medicine, GA, USA (2007~2011); Full Professor in Graduate School of Nutritional Sciences, University of Shizuoka, Shizuoka, Japan (1993 ~ 2007); Associate Professor in Graduate School of Nutritional Sciences, University of Shizuoka, Shizuoka, Japan (1991~1993); Assistant Professor in School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka, Japan (1987~1991); Research Associate in Shizuoka College of Pharmacy, Shizuoka, Japan (1973 ~ 1986). He received a Ph.D. in Pharmaceutical Sciences from Shizuoka College of Pharmacy Shizuoka, Japan (1976). He has completed his M.S. (1973) and B.S. (1971) in Pharmaceutical Sciences, Shizuoka College of Pharmacy, Shizuoka, Japan).

Professional membership. *Editorial Academy Member in International Journal of Molecular Medicine (2001-2019); Editorial Board Member in Molecular and Cellular Biochemistry (2010-2013); Editorial Academy Member in International Journal of Oncology (2015-2019); Editorial Board Member in Current Molecular Medicine (2019 -); Section Editor in the Editorial Board Member of Current Nutraceuticals (2019); Editorial Board Member in Cancers (2020); Editorial Board Member of Translational Oncology (2021-); Co-Editors of Current Cancer Drug Targets (2021 -).*

Membership in professional organizations*. Dr. Yamaguchi serviced with the membership in Professional Organizations, including Japan Society for Pharmaceutical Sciences (1971 – 2011), Japan Society for Biochemistry, Councilor (1973 – 2011), Endocrine Society for Japan, Councilor (1977 – 2010), International Society of Bone and Mineral (1984 – 2007), Japan Society for Pharmacology, Councilor (1987 – 2007), Japan Society for Bone and Mineral Metabolism, Councilor (1988 – 2007), Japan Society for Biomedical Research on Trace Elements, Councilor (1990 – 2011), Japan Society for Hepatocyte Research, Councilor (1995 – 2006), European Society of Calcium (1997 – 2004), Japan Society for Osteoporosis, Councilor (1999 – 2008), American Society for Cell Biology (2001 – 2007), The New York Academy of Sciences (1996 – 2012), American Society for Bone and Mineral Research (1999 – 2017), American Society for Biochemistry and Molecular Biology (2005 -),European Union (EU) Academy of Sciences (2021 -).*

Awards and Honors*. Dr. Yamaguchi received many honors and awards, including Prize for Sato Memorial Foundation (1992, Japan/USA); Senji Miyata Foundation Award 2005, Japan; Japan Society for Biomedical Research on Trace Elements Award, Japan, 2007; The Lifetime*

Achievement Award from International Biographical Centre (IBC), Cambridge, UK (2004); The World Lifetime Achievement Award from American Biographical Institute, USA (2004); The Distinguished Service to Science Award IBC, Cambridge, UK (2007) and many others. Dr. Yamaguchi is listed in various biographies; Who's Who in the World (2005-, Marquis Who's Who, USA), Who's Who in Sciences and Engineering (2004-, Marquis Who's Who, USA), International Biographical Dictionary (2006, IBC, UK), Who's Who in America (2009-, Marquis Who's Who, USA), and Who's Who in Asia (2007-, Marquis Who's Who, USA). Notably, Dr. Yamaguchi received "The 2017 Albert Nelson Marquis Lifetime Achievement Award (Marquis Who's Who, USA).

Contribution to Science

Dr. Yamaguchi is engaged in the fields of endocrinology and cell signaling since 1971, and these researches are developed in the diverse aspects of biochemistry, molecular biology, endocrinology, metabolism, nutrition, pharmacology, and toxicology. In recent years, Dr. Yamaguchi is impressively interested for cell signaling mechanism, bone biology, osteoporosis prevention, cancer biology, cancer bone metastasis and treatment. Moreover, Dr. Yamaguchi discovered two novel proteins and genes; cell signaling suppressor protein (named regucalcin; 1978) and transcriptional factor RGPR-p117 (regucalcin gene promoter region-related protein; 2001, renamed to SEC16B in 2007) in mammalian cells. Dr. Yamaguchi demonstrates that regucalcin plays a crucial role as a suppressor in carcinogenesis of patients with various types of human cancers. Currently, the research of regucalcin is focused as scientific topics worldwide. Dr. Yamaguchi published 589 English articles in professional journals with peer-review. Dr. Yamaguchi registered 27 national and international patents in the fields of his research interesting. Moreover, Dr. Yamaguchi is served as editorial board members of over 90 international Journals.

Studies on calcium and bone metabolism

In study of aging, calcium and bone metabolism were attractively paid attention in the field of endocrinology and biomedical sciences. In 1975, Dr. Yamaguchi found that the liver was a target organ of calcitonin, a calcium-regulating hormone, that has a physiologic hypocalcemic effect in blood calcium homeostasis. In this connection, Dr. Yamaguchi elucidate a novel metabolic pathway that serum calcium is transported into liver cells and is excreted into the hepatic bile duct and intestine. Calcitonin was found to stimulate transport of calcium into liver cells and promoted excretion into the bile of increased liver calcium by using rat model in vivo. This metabolic pathway played a physiologic role in regulation of hypercalcemia after intake of dietary calcium. Furthermore, Dr. Yamaguchi participate in the field of bone biology for longer years. Ahead of the world, Dr. Yamaguchi elucidated the role of various nutritional factors in regulation of osteoblasogenesis and osteoclastogenesis and in prevention and therapy of osteoporosis with aging. In recent years, Dr. Yamaguchi contributed to research of bone metabolic disorders, including HIV-1 and cancer bone metastasis. *Partly related publications: Yamaguchi M, Takei Y, Yamamoto T: Effect of thyrocalcitonin on calcium concentration in liver of intact and thyroparathyroidectomized rats. Endocrinology, 96: 1004-1008 (1975); Yamaguchi M, Oishi H, Suketa Y: Stimulatory effect of zinc on bone formation in tissue culture. Biochemical Pharmacology, 36:4007-4012 (1987); Yamaguchi M, Zhu S, Zhang S, Wu D, Moore TM, Snyder JP, Shoji M: Curcumin analogue UBS109 prevents bone loss in*

breast cancer bone metastasis mouse model: Involvement in osteoblastogenesis and osteoclastogenesis. Cell and Tissue Research, 357:245-252 (2014); Ofotokun I, Titanji K, Vikulina T, Roser-Page S, Yamaguchi M, Zayzafoon M, Williams IR, Weitzmann MN: Role of T cell reconstitution in HIV-1 antiretroviral therapy-induced bone loss. Nature Communications 6:8282 (2015). Doi:10.1038/ncomms9282.

Discovery of regucalcin and identification of its related transcriptional factors

In process of the studies of calcium metabolic pathway as mentioned above, Dr. Yamaguchi discovered a novel calcium-binding protein, regucalcin (gene symbol; *rgn*), which contains no EF-hand motif of Ca^{2+}-binding domain. The name, regucalcin, was proposed for this Ca^{2+}-binding protein, which can regulate activities of various Ca^{2+}-dependent enzymes in cells. Dr. Yamaguchi et al. identified structure of regucalcin in various vertebrate specifies, including human, and found that the regucalcin gene localized on the X chromosome, and identified the 5'end sequences and organization in the regucalcin gene consists of seven exons and six introns. Furthermore, Dr. Yamaguchi et al identified that the regucalcin gene expression was regulated by various transcription factors, including AP-1, NF1-A1, RGPR-p117 and other factors, which are modulated via intracellular signaling factors implicated in phosphorylation and dephosphorylation of nuclear protein. Discovery of regucalcin is impressively contributed in sciences. *Related publications: Yamaguchi M, Yamamoto T: Purification of calcium binding substance from soluble fraction of normal rat liver. Chemical & Pharmaceutical Bulletin (Tokyo), 26:1915-1918 (1978). Doi: 10.1248/cpb.26.1915; Shimokawa N, Yamaguchi M: Molecular cloning and sequencing of the cDNA coding for a calcium-binding protein regucalcin from rat liver. FEBS Lett 327: 251-255 (1993); Shimokawa N, Matsuda Y, Yamaguchi M: Genomic cloning and chromosomal assigment of rat regucalcin gene. Molecular and Cellular Biochemistry, 151:157-163 (1995); Murata T, Yamaguchi M: Promoter characterization of rat gene for Ca^{2+}-binding protein regucalcin. Journal of Biological Chemistry, 274:1277-1285 (1999).*

Discovery of novel transcription factor RGPR-p117

In process of the studies of transcriptional regulation of the regucalcin gene expression, Dr. Yamaguchi et al originally discovered as a novel protein, named as RGPR-p117 (gene symbol, *rgpr-p117*), which binds to a nuclear factor I (NFI) consensus motif $TTGGC(N)_6CC$ that is present in the promoter region of the regucalcin gene. Dr. Yamaguchi et al found that RGPR-p117 was expressed in human and other species with a common evolutionary relationship of the RGPR-p117 family. Also, Dr. Yamaguchi et al identified that the RGPR-p117 gene consisted of 26 exons spanning approximately 4.1 kbp and was localized on human chromosome 1q25.2. Dr. Yamaguchi et al found that phosphorylated RGPR-p117 was translocated via signaling process that was mediated by activation of protein kinase C. Furthermore, Dr. Yamaguchi et al found that overexpression of RGPR-p117 suppressed the gene expressions of various proteins of whose TTGGC motif was present in the promoter region of their genes. RGPR-p117 is proposed to play a crucial role as a novel transcription factor. In 2007, RGPR-p117 was renamed as SEC 16 homolog B (SEC16B; PubMed)). *Related publications: Misawa H, Yamaguchi M: Molecular cloning and sequencing of the cDNA coding for a novel regucalcin gene promoter region-related protein in rat, mouse and human liver. International Journal of Molecular Medicine 8: 513-520 (2001); Sawada N, Nakagawa T, Murata T, Yamaguchi*

M: Nuclear localization of a novel protein, RGPR-p117, in cloned normal rat kidney proximal tubular epithelial cells. International Journal of Molecular Medicine, 16: 809-814 (2005); Sawada N, Yamaguchi M: Overexpression of RGPR-p117 enhances regucalcin gene promoter activity in cloned normal rat kidney proximal tubular epithelial cells: Involvement of TTGGC motif. Journal of Cellular Biochemistry 99: 589-597 (2006); Yamaguchi M: Novel protein RGPR-p117: its role as the regucalcin gene transcription factor. Molecular and Cellular Biochemistry 327:53-63 (2009) (Review).

Role of regucalcin in cell regulation and metabolic disorder

Since discovery of regucalcin, Dr. Yamaguchi investigate that regucalcin plays a multifunctional role in regulation of cellular function in various types of cells. Regucalcin is found to regulate intracellular Ca^{2+} homeostasis and activity of various enzymes, including protein kinases, protein phosphatases, nitric oxide synthase, cysteinyl proteases, aminoacyl-tRNA synthetase, and others. Of note, Dr. Yamaguchi et al found that the cytoplasmic regucalcin was translocated into the nucleus underling mechanism by which is mediated via signaling process of activated protein kinase C. Furthermore, Dr. Yamaguchi et al determined that nuclear regucalcin binds to nuclear DNA and protein, leading to inhibition of nuclear Ca^{2+}-dependent and -independent protein kinases and protein phosphatases, Ca^{2+}-activated DNA fragmentation, and DNA and RNA syntheses. Importantly, regucalcin was found to regulate the gene expression of various proteins, indicating a role as a novel transcription factor. Moreover, regucalcin was found to be suppressed cell proliferation and increased apoptosis. Importantly, regucalcin was found to induce G1 and G2/M phase cell cycle arrest. Thus, Dr. Yamaguchi elucidates that regucalcin plays a pivotal role in regulation of cellular function. Furthermore, Dr. Yamaguchi et al investigated a pathophysiologic role of regucalcin in metabolic disorder by generating regucalcin transgenic (TG) rats. Dr. Yamaguchi et al found that osteoporosis and hyperlipidemia were caused in the TG rats with increasing aging in vivo. In the TG animal models, Dr. Yamaguchi et al investigated the mechanism by which regucalcin TG rats induced osteoporosis due to stimulating osteoclastic bone resorption and suppressing osteoblastic bone formation, supporting a role of regucalcin in bone homeostasis and bone remodeling. In addition, Dr. Yamaguchi et al found that hyperlipidemia, hyperalbumia and hypercalcemia are induced in regucalcin TG rats with increasing age. Interestingly, overexpression of regucalcin was found to lead to insulin resistance in liver cells due to stimulating glucose transporter 2 mRNA expression and suppressing insulin receptor and phosphatidylinositol 3-kinase mRNA expressions involved in insulin signaling. Thus, regucalcin TG rat model is proposed to be a useful animal model as therapeutic tool for osteoporosis and hyperlipidemia. Dr. Yamaguchi registered International Patent in USA, Japan, EU, and Korea (Title: Model animal with overexpression of regucalcin. United States Patent 7,355,093 B2, registered April 8, 2008; Inventor: Yamaguchi M. Assignee: Japan Science and Technology Agency, Japan).

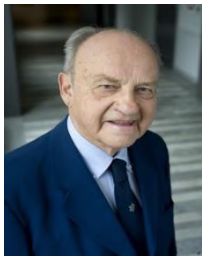
Related publications: Yamaguchi M: Role of regucalcin in calcium signaling. Life Sciences 66:1769-1780 (2000) (Review); Yamaguchi M: Role of regucalcin in maintaining cell homeostasis and function (Review). International Journal of Molecular Medicine, 15: 371-389 (2005); Yamaguchi M: Role of regucalcin in cell nuclear regulation: Involvement as a transcription factor. Cell and Tissue Research 354:331-341(2013) (Review); Yamaguchi M, Murata T: Involvement of regucalcin in lipid metabolism and diabetes. Metabolism Clinical and Experimental 62:1045-1051(2013) (Review).

Role of regucalcin as a novel suppressor in human cancer

Regucalcin plays a crucial role as an inhibitory protein in signaling processes linked to cell growth. Since 2013, Dr. Yamaguchi focuses on cancer research to elucidate a potential role of regucalcin as a suppressor in cell growth and carcinogenesis. Notably, many studies with proteomics and multiple gene expression profiles demonstrate that the regucalcin gene expression and its protein levels are uniquely downregulated in the tumor tissues of various types of human cancer patients. These decreases were associated with progression of carcinogenesis in human cancer patients, and survival of patients was prolonged with higher levels of regucalcin in the tumor tissues of patients, including pancreatic cancer, breast cancer, liver cancer, lung cancer, colorectal cancer, renal cancer, and prostate cancer. Moreover, our translational studies demonstrated that overexpressed regucalcin suppressed the proliferation of human cancer cells, including pancreatic cancer MIA PaCa-2 cells, MDA-MB-231 breast cancer cells, liver cancer HepG2 cells, lung adenocarcinoma A549 cells, colorectal cancer RKO cells, renal cell carcinoma A498 cells, osteosarcoma Saos-2 cells, and prostate cancer PC-3 and DU-145 cells in vitro. Thus, regucalcin was demonstrated to play a pivotal role as a suppressor in various type of human cancer. Downregulated regucalcin gene expression may contribute to malignancies of human subjects. We propose that delivery system with the regucalcin gene is useful as a novel therapeutic tool in human cancer treatment. *Related publications:* *Yamaguchi M: Suppressive role of regucalcin in liver cell proliferation: Involvement in carcinogenesis. Cell Proliferation 46:243-253(2013) (Review); Yamaguchi M: Involvement of regucalcin as a suppressor protein in human carcinogenesis: Insight into the gene therapy. Journal of Cancer Research and Clinical Oncology, 1333-1341 (2013) (Review); Yamaguchi M, Osuka S, Murata T: Prolonged survival of colorectal cancer patients is associated with a higher regucalcin gene expression: Overexpressed regucalcin suppresses growth of human colorectal carcinoma cells in vitro. International Journal of Oncology, 53:1313-1322 (2018); Yamaguchi M, Osuka S, Murata T, Ramos JW: Progression-free survival of prostate cancer patients is prolonged with a higher regucalcin expression in the tumor tissues: Overexpressed regucalcin suppresses the growth and bone metastatic activity of PC-3 cells in vitro. Translational Oncology 14: 10095 (2021). doi.10.1016/j.tranon.2020.100955.*

Potentialities of a Subatomic Theory

by Bo Lehnert, Member EUAS



Short Biography

Born in Stockholm, Sweden, on March 30 in 1926.
Doctoral degree at Royal Institute of Technology, Stockholm 1955. Full Professor, Personal Chair of Swedish Atomic Research Council in 1968. Head of Plasma Physics Division of European Physical Society 1969-1972. Member of International Fusion Research Council of the International Atomic Energy Agency, Vienna, in 1970–1991.
Fellow of Institute of Mathematics and its Applications, London, 1973, member of Royal Swedish Academy of Sciences 1974, of Royal Swedish Academy of Engineering Sciences 1975, of the Electromagnetics Academy, Cambridge, Mass. USA, 1980. Original contributions in international journals on magnetohydrodynamics, plasma physics, thermonuclear fusion, revised quantum electrodynamics and subatomic physics, with five books in these fields.
Recipient of Edlund Prize of Royal Swedish Academy of Sciences, of Celsius Gold Medal of the Science Society in Uppsala, and of the Medal of His Majesty the King of Sweden.

Abstract

A condensed summary is given of the manifold of new results which originate from a subatomic theory, based on the concepts of Zero Point Energy and nonzero quantum fluctuations with electric charge density in the vacuum. These results include models of the photon and electron, a new version of the Higgs boson, a strong force deduced from interactions between intrinsic electric charges, a new consideration on the contradiction between quantum mechanics and relativity, and of a finite characteristic radius of black holes.

1. Introduction

The properties of elementary particles have earlier been discussed by the author in terms of subatomic physics [1–4]. A fundamental part of this theory is due to the contribution from Zero Point Energy [5], as given by a lowest nonzero level of the Planck energy of the harmonic oscillator [6]. Consequently, the vacuum state is not merely that of an empty space but includes quantum fluctuations, as shown by Casimir [7] and first demonstrated experimentally by Lamoreaux [8]. Part of the fluctuations carry electric charge, as pointed out by Abbott [9].

These properties have been considered in connection with the concepts of particle rest mass, spin, elementary and intrinsic electric charges, needle radiation, the strong force, the

binding energy of neutrons and protons, the Higgs mass, the relation between quantum mechanics and relativity, and the characteristic radius of a black hole. Here the basic features of the theory will be reconsidered in a condensed and shortened form.

2. Divergency of the Field Strengths

2.1 Magnetic Field

Due to all so far made experience, isolated magnetic monopoles do not exist in nature. An example is given by the investigations of the photospheric magnetic field of the sun by Babcock and Babcock [10]. These include the so-called unipolar magnetic (UM) regions having only one polarity. But such regions cannot be taken as an indication of existing magnetic monopoles, because it is not apparent where the emergent magnetic field returns to the sun.

Thus all theoretical concepts can be based on a divergence-free magnetic field strength **B**, with div $\mathbf{B} = 0$.

2.2 Electric Field

2.2.1 Zero Divergency

A strongly restricted situation arises in subatomic physics when attempts are made to treat the *interior* of an elementary particle under the subsidiary condition of a vanishing div **E**. This leads to severe shortcomings such as a vanishing spin of a propagating photon being in contradiction with experiments, as well as a symmetry between the fields **E** and **B,** which results in a lacking particle-like photon state [2–4].

2.2.2 Nonzero Divergency

An extended electromagnetic theory has been elaborated on the basis of a nonzero local charge density $\bar{\rho} = \varepsilon_0 \operatorname{div} \mathbf{E}$ in the vacuum. The corresponding four-dimensional form of the electromagnetic field equations becomes [1–4]

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right) A_\mu = \mu_0 J_\mu \tag{1}$$

with: μ = 1,2,3,4,

$$A_\mu = (\mathbf{A}, i\varphi/c) \tag{2}$$

where **A** and φ are the magnetic vector potential and the electrostatic potential, and

$$J_\mu = (\mathbf{j}, ic\bar{\rho}) \tag{3}$$

is a four-current density where **j** stands for the three-space current density and $\bar{\rho}$ for the charge density. Due to the Lorentz invariance

$$J_\mu = \bar{\rho}\,(\mathbf{C}, ic) \tag{4}$$

where:

$$\mathbf{C^2} = c^2 = 1/\varepsilon_0\mu_0 \tag{5}$$

and **C** stands for a *velocity vector* with a modulus equal to the *velocity constant c* of light. This replacement of *c* by **C** is due to an extension of the photon wave representation of special relativity to a three-dimensional one, such as that of cylindrical geometry with an *incorporated* spin concept in addition to the main photon propagation. Needless to say, the concept of special relativity by Einstein still holds with this incorporation.

As a result, the three-dimensional representation of the extended subatomic field equations of the *vacuum* state becomes

$$\text{curl}\,\mathbf{B}/\mu_0 = \varepsilon_0\,(\text{div}\,\mathbf{E})\,\mathbf{C} + \varepsilon_0\frac{\partial \mathbf{B}}{\partial t} \tag{6}$$

$$\text{curl}\,\mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{7}$$

with

$$\mathbf{B} = \text{curl}\,\mathbf{A}\,, \qquad \text{div}\,\mathbf{B} = 0 \tag{8}$$

$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}\,, \qquad \text{div}\,\mathbf{E} = \bar{\rho}/\varepsilon_0 \tag{9}$$

Three limiting cases can in principle be identified on the basis of the present field equations:

- When $\text{div}\,\mathbf{E} = 0$ and $\text{curl}\,\mathbf{E} \neq 0$ there is a conventional transverse electromagnetic wave, here denoted as an "EM wave".
- When $\text{div}\,\mathbf{E} \neq 0$ and $\text{curl}\,\mathbf{E} = 0$ there is a purely longitudinal electric spacecharge wave, here denoted as an "S wave".
- When both $\text{div}\,\mathbf{E} \neq 0$ and $\text{curl}\,\mathbf{E} \neq 0$ a hybrid nontransverse electro-magnetic space-charge wave appears, here denoted as an "EMS wave".

An important particular case is that of steady axisymmetric states in a frame (r, θ, φ) of spherical coordinates where all quantities are independent of the angle φ. Then the current density becomes $\mathbf{j} = (0, 0, C\bar{\rho})$ where $C = \pm c$ represents the two spin directions, and the magnetic vector potential in three-space becomes $\mathbf{A} = (0, 0, A)$. The field equations (6)–(9) then combine to a basic equation having a general solution obtained in terms of a *generating function*

$$F(r, \theta) \;=\; CA - \phi \;=\; G_0 \cdot G(\rho, \theta) \tag{10}$$

with $\rho \;=\; r/r_0$ and where G_0 stands for a characteristic amplitude and G for a normalized part. This yields a general solution

$$CA = -(\sin\theta)^2 DF \tag{11}$$

$$\phi = -[1 + (\sin\theta)^2 D]F \tag{12}$$

$$\bar{\rho} = -(\varepsilon_0/r_0^2\rho^2)\; D\;[1 + (\sin\theta)^2 D]F \tag{13}$$

for the potentials $(\mathbf{A}, i\phi/c)$, the charge density $\bar{\rho}$, and D standing for an operator [1].

3. The Charge Density in Subatomic Physics

A nonzero electric charge density forms the basis of a number of new aspects in subatomic physics.

3.1 Cylindrical Photon Model

With Equations (6)–(9) in a cylindrical frame the velocity vector

$$\mathbf{C} = c(0, \cos\alpha, \sin\alpha) \tag{14}$$

where α is a constant angle. Here $\sin\alpha > 0$ and is slightly smaller than unity. It represents a propagating part in the forward direction. Further $0 < \cos\alpha \ll 1$ represents the spin motion in the transverse direction. A *generating function*

$$F(r, z, t) = G_0 \cdot G = E_z + (\cot\alpha)E_\varphi \tag{15}$$

with:

$$G = R(\rho)\, e^{i(-\omega t + kz)} \tag{16}$$

can then be introduced with $R(\rho)$ as a *convergent* radial part [1]. For axisymmetric photon wave packets the positive and negative spatial contributions to the electric charge density will then become differently distributed in space, but the total integrated electric charge and magnetic moment will *vanish*.

There is also a photon mode originating from a generating function with a *divergent* radial part, combined with an *antisymmetric* polar part. Also this results in a *vanishing* integrated electric charge. A revised renormalization procedure then leads to finite properties in the form of *needle radiation*.

3.2 Electron Model

According to Equations (6)–(9) a *net* integrated electric charge only becomes possible when the radial part of the generating function becomes *divergent*. Still a limited charge can be obtained through a revised renormalization procedure. This leads to a *point-charge-like* system [1–4].

3.3 Intrinsic Charges

The local nonzero div $\mathbf{E}$ does not only give rise to a net integrated charge, but also to *intrinsic* integrated electric charges $\pm Q$ of both polarities within *various* parts of an elementary particle [1–4,11]. Here a model has been elaborated of quarks which form triangular neutron and positron configurations. These “quark particles” are electrically neutral as an entity, but contain charges of both polarities, being an order of magnitude *larger* than the elementary charge. They originate from a *convergent* generating function.

4. New Results from Subatomic Theory

The present subatomic theory has resulted in a number of new fundamental results which also have been confirmed experimentally [1–4,11,12].

4.1 The Photon

Cylindrical waves with a velocity vector of Equation (14) lead to a screw-shaped configuration which includes spin and an associated very small but nonzero photon *rest*

mass. The phase and group velocities become slightly smaller than *c*, the field geometry is *helical* with axial field components, and the photon configuration becomes *limited* in space.

4.2 The Elementary Charge

For divergent models of the electron, muon and tauon a revised renormalization procedure results in a net electric charge $q_0 = Q_0 f_p$ where $Q_0 = (\varepsilon_0 ch)^{1/2} \cong 8.86 \times 10^{-19}$ C and f_p is a dimensionless profile factor. A variational analysis on f_p further results in a *minimum* charge $q_0 \cong 1.60 \times 10^{-19}$ C, being close to the experimental value of the elementary charge. It suggests that this charge should be conceived as a deduced quantity, and not as an independent parameter. This is consistent with the deduction by von Klitzing [13] of the unit charge of the electron in a *two-dimensional* electron gas.

4.3 The Higgs Particle

In a theory by Higgs [14] on symmetry breaking of an empty vacuum state, an unstable boson of unspecified but large rest mass, zero net electric charge and zero spin is being deduced. Later a similar particle was detected at the projects ATLAS [15] and CMS [16] of CERN, being unstable and having a rest mess of 125 GeV.

A different way of explaining the result of CERN has been presented by the author [17–19]. It starts with the superposition of two bosons with antiparallel spin directions, each with a mass of 91 GeV. The resulting composite particle then has zero electric charge, magnetic field and spin, is purely electrostatic and highly unstable, and has a minimum mass close to the observed value of 125 GeV.

4.4 The Strong Force

The interaction between two quarks in the model described here in terms of the intrinsic electric charges can be summarized as follows [2,4,11]:

- This interaction is of *short-range* character, and becomes *two* orders of magnitude larger than that between two elementary charges.
- When gradually shrinking the distance between two quark centra, the corresponding work by the mutual force results in an outer potential barrier, followed by an intermediate well, and ending at an additional barrier. The mutual quark interaction thus becomes *stable* and *attractive*.
- An application to the neutron leads to a well depth of about 7.7 MeV, being close to the binding energy of 8 MeV reported by Bethe [20].

4.5 Special Relativity and Quantum Mechanics

In quantum mechanics an instantaneous interaction can take place through longrange forces. This appears not to be reconcilable with limited relativistic propagation of conventional electromagnetic waves. A way out of this contradiction may be provided by a multistage procedure applied to the modes of the subatomic field equations (6)–(9). First, there is an EMS nontransverse space-charge mode with a limited relativistic propagation by the velocity vector. Second, there is also included an S mode of purely longitudinal

electric space-charge character. The latter mode depends only on the dielectric constant ε_0 and not on μ_0. It has no direct relation to relativity and its velocity of propagation. A combination of these modes could solve this problem, but requires further consideration.

4.6 Characteristic Radius of Black Holes

The force balance during the final state of black holes is conceived to be governed by the Zero Point Energy [12]. This makes a force balance possible at a *finite* characteristic radius of a black hole mass distribution.

5. Conclusions

A manifold of new fundamental results have been deduced from a subatomic theory, not being available from conventional investigations. These include modified models of the photon and electron, a new version of the Higgs boson, a strong force deduced from intrinsic electrodynamic charge interaction, a possible resolution of the contradiction between quantum mechanics and relativity, and a finite obtained characteristic radius of black holes.

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Behavioral Traits that define Social Dominance are the same that reduce Social Influence in a Consensus Task

by Oliver Deussen, Member EUAS

Short Biography

Education and Professional Experience

Mar 2003 – now	***Full Professor***
	Visual Computing, Konstanz University, Germany
Jun 2010 – Dec 2020	***Visiting Professor***
	Shenzhen Institute of Applied Technologies, Chinese Academy of Science, China
Jul – Sep 2006	***Visiting Researcher***
	Computer Graphics Group, Microsoft Research, Redmond
Mar 2004 – Sep 2005	***Head of Department***
	Computer and Information Science, Konstanz University, Germany
Sep 2000 – Feb 2003	***Associate Professor (C3)***
	Dresden University of Technology, Germany
Apr 1996 – Aug 2000	***Postdoctoral Researcher***
	Otto-von-Guericke University of Magdeburg, Germany
Mar 1996	***Graduation***
	Dr. rer nat, Karlsruhe Institute of Technology (KIT), Germany

Professional Activities

Jan 2019 – now	***Speaker***
	Excellence Cluster "Centre for the Advanced Study of Collective Behaviour", University of Konstanz (with Iain Couzin and Urs Fischbacher)
Jan 2019 – Dec 2020	***President***
	Eurographics Association
Jan 2012 – Dec 2015	***Editor in Chief***
	Computer Graphics Forum, Journal for Computer Graphics
Jul 2015 – now	***Vice Speaker***
	DFG Collaborative Research Center 161 Quantitative Methods for Visual Computing with Daniel Weiskopf, University of Stuttgart
March 2020 – now	***DFG Review Board***
	DFG Review Board 409-05 "Interactive and Intelligent Systems, Image and Language Processing, Computer Graphics and Visualization"
Ongoing	***Associated Editor, IPC-Member, Papers Chair etc.***
	ACM SIGGRAPH; IEEE Visualization; Eurographics; Pacific Graphics; Workshop on Computational Aesthetics in Graphics,

	Visualization and Imaging; Symposium on Non-Photorealistic Animation and Rendering; Vision Modelling Visualization; Informatik Spektrum; Sibgrapi; Sino-German Symposium on Visualization, Selection committees for Studienstiftung des Deutschen Volkes

Honors, Awards, Patents, Scientific Achievements

2020	*Member EU Academy of Sciences*
2016	*awarded within the Guangdong leading Talents Plan (China)*
2014	*awarded within the 1000 Talents Plan (China)*
2014	*Nomination Technical Achievement Award for Xfrog Modelling Software*
2013	*Eurographics Fellow*
2007	*awarded Virtual earth academic collaboration of Microsoft Research, 35k USD*

Ten important Publications

1. Mariana Rodriguez-Santiago, Paul Nührenberg, James Derry, Oliver Deussen, Fritz A Francisco, Linda K Garrison, Sylvia F Garza, Hans A Hofmann, and Alex Jordan. **Behavioral traits that define social dominance are the same that reduce social influence in a consensus task**. Proceedings of the National Academy of Sciences (PNAS), 117(31):18566–18573, 2020

   A first high-profile paper within our Excellence Cluster. We contributed tracking methods and visual analysis. The paper shows that fish swarms learn less from dominant males than from less dominant and more social exemplars

2. Jörg Marvin Gülzow, Patrick Paetzold, and Oliver Deussen. **Recent developments regarding painting robots for research in automatic painting, artificial creativity, and machine learning**. Applied Sciences, 10(10):3396, 2020

   The latest paper of our e-david project in which we develop a painting robot that, like human painters, uses visual feedback to create its paintings. The machine is able to paint with acrylic colors and handle a variety of brushes.

3. Spicker M., F. Götz-Hahn, T. Lindemeier, D. Saupe, O. Deussen: **Quantifying Visual Abstraction Quality for Computer-Generated Illustrations,** *ACM Transactions on Applied Perception 16.1 (2019), P. 5:1-20*

   This paper is the first that quantitatively measures visual abstraction, here for the case of stippling, a dot-oriented abstraction method. We show that the Weber-Fechtner law applies here and can be used to quantify the perceived visual abstraction of a stipple drawing.

4. Deussen O., M. Spicker, Q. Zheng*:* **Weighted Linde-Buzo-Gray Stippling,** ACM Transactions on Graphics 36.6 (2017), P. 233:1-12

   We present an improvement of a popular algorithm for automatic abstraction (stippling) that enables to create abstractions automatically based on some simple optimization criteria.

5. Ahmed, G., Perrier, H., Coeurjolly, D., Ostromoukhov, V., Guo, J., Yan, D., Huang, H., and Deussen, O.: **Low-Discrepancy Blue Noise Sampling,** ACM Transactions on Graphics (TOG) 35 (6), 247, 2016

   We present the first method to create Blue Noise point distributions (very important for sampling in Computer Graphics) based on discrete, easy and fast to produce processes with low discrepancy.

6. Liangliang Nan, Andrei Sharf, Ke Xie, Tien-Tsin Wong, Oliver Deussen, Daniel Cohen-Or, and Baoquan Chen. **Conjoining gestalt rules for abstraction of architectural drawings**. ACM Transactions on Graphics (TOG), 30(6):1–10, 2011.

   Gestalt laws are very popular in psychology, but they are not real laws since they cannot predict much. Some of these laws, however, can be mathematically formulated and be used for visual abstraction. This paper is the first that allows this by using multi-graph cuts to deal with conflicting laws.

7. Heino Hellwig, Ralph Engelmann, and Oliver Deussen. **Contact pressure models for spiral phyllotaxis and their computer simulation**. Journal of Theoretical Biology, 240(3):489–500, 2006

   My most underrated paper. We present the first simulation method for complex seed arrangements in sun flowers and other plants that, based on Voronoi Diagrams, exhibit the Golden Section arrangement including existing statistical deviations based on simple biological start conditions. This method explains the beauty of seed (and petal arrangements) in nature.

8. Michael Balzer and Oliver Deussen. **Voronoi treemaps**. In IEEE Symposium on Information Visualization (INFOVIS 2005), PP 49–56. IEEE Association, 2005

   We developed a popular Visualization Technique called Voronoi Treemaps, which today is widely used in science and also popular media for displaying hierarchical data sets.

9. Michael F Cohen, Jonathan Shade, Stefan Hiller, and Oliver Deussen. **Wang tiles for image and texture generation**. ACM Transactions on Graphics (TOG), 22(3):287–294, 2003

Placing objects in Computer Graphics suffers from repetition artifacts, especially when large scenes are shown in perspective projection. We introduce Wang Tiles, a simple non-repetitive arrangement method known from mathematics, for placing objects and for texture synthesis.

10. Bernd Lintermann and Oliver Deussen. **Interactive modeling of plants**. IEEE Computer Graphics and Applications, 19(1):56–65, 1999.

An interactive modelling method that for the first time combines rule-based modelling with parameterized components and this way allows to create complex plant models efficiently. The approach initiated the development of companies such as Xfrog, Inc. and Laubwerk (a Berlin-based company) and was nominated for the technical achievement award (technical Oscar of the Academy for Motion Picture Arts).

American Society of Hematology Guidelines for Management of Venous Thromboembolism

by Ian A. Greer, Member EUAS

Short Biography

Qualifications *MBChB 1980, MD (Glasgow) 1986, MRCP(UK) 1984, FRCP(Glas) 1994, FRCPE 1999, FRCP 2001, FRCPI 2006 MFFP 1994, FFFP 2007, FFSRH 2009. MRCOG 1987, FRCOG 1999 FAE 2003 FMedSci 2006 FCCP 2011*

Professional and Academic Appointments

From 2018 *President & Vice Chancellor, Queen's University, Belfast.*
From 2020 *Council Member - Research England, UKRI*
Non-remunerated Positions
From 2018 *Chair, Innovation Pillar Board, Belfast Region City Deal*
From 2019 *Non-Executive Director and founder, Health Innovation Research Alliance, Northern Ireland*
From 2019 *Member, Board of Trustees Mohammed Bin Rashid University, UAE*
From 2020 *President, Universities Ireland*

Major Awards and Honours

MRCOG Gold Medal
William Blair Bell Memorial Lectureship of the Royal College of Obstetricians and Gynaecologists,
Bernhard Baron Travelling Scholarship of the Royal College of Obstetricians and Gynaecologists, at the Lawson Research Institute, University of Western Ontario, London, Ontario, Canada.
Watson Prize Lectureship of the Royal College of Physicians and Surgeons of Glasgow.
Manchester Medal, Royal College of Physicians of Edinburgh
Honor of Guest Professor, Peking University Health Sciences Center 2017-19
Deputy Lieutenant Co Borough of Belfast

Research Advisory Boards & Committees and Grant Reviewing

Medical Research Council
Member, Translational Research Group (2015-)
Chair, Quinquennial Review, MRC/Wellcome Trust Cambridge Stem Cell Institute (2016)
Chair, Translational Stem Cell Research/Regenerative Medicine Committee (2008-2014)
Member, Translational Research Group (2008-2011)
Member, Review Group for the MRC Human Reproductive Sciences Unit, (2010)

Deputy Chair, Physiological Systems & Clinical Sciences Board (2006-8) (Member 2004-6)
Member, Strategic Portfolio Overview Group, Physiological Systems & Clinical Sciences Board (2006-8)
Chair, Pilot Industry Awards Panel (2008)
Member, IES Platforms Panel (2008)
Member, Biomarkers Awards Panel (2007)
Member, Cross Board Group for Clinical Trials. (2005-8)
Member, Review Group for the MRC Centre for Reproductive Biology (2004)
Member, MRC Virucides Advisory Committee (2003-4)
Member, Medical Research Council, Medical Advisory Board (2000-2004)
Member, Medical Research Council Expert Team of Research Training Referees (2000-4)

TOP PUBLICATIONS

1. Blood Adv. 2018 Nov 27;2(22):3317-3359. doi: 10.1182/bloodadvances.2018024802.

American Society of Hematology 2018 guidelines for management of venous thromboembolism: venous thromboembolism in the context of pregnancy.

Bates SM(1)(2), Rajasekhar A(3), Middeldorp S(4), McLintock C(5), Rodger MA(6)(7)(8), James AH(9), Vazquez SR(10), Greer IA(11), Riva JJ(12)(13), Bhatt M(13), Schwab N(14), Barrett D(15), LaHaye A(16), Rochwerg B(13)(17).

BACKGROUND: Venous thromboembolism (VTE) complicates ~1.2 of every 1000 deliveries. Despite these low absolute risks, pregnancy-associated VTE is a leading cause of maternal morbidity and mortality. OBJECTIVE: These evidence-based guidelines of the American Society of Hematology (ASH) are intended to support patients, clinicians and others in decisions about the prevention and management of pregnancy-associated VTE. METHODS: ASH formed a multidisciplinary guideline panel balanced to minimize potential bias from conflicts of interest. The McMaster University GRADE Centre supported the guideline development process, including updating or performing systematic evidence reviews. The panel prioritized clinical questions and outcomes according to their importance for clinicians and patients. The Grading of Recommendations Assessment, Development and Evaluation (GRADE) approach was used to assess evidence and make recommendations. RESULTS: The panel agreed on 31 recommendations related to the treatment of VTE and superficial vein thrombosis, diagnosis of VTE, and thrombosis prophylaxis. CONCLUSIONS: There was a strong recommendation for low-molecular-weight heparin (LWMH) over unfractionated heparin for acute VTE. Most recommendations were conditional, including those for either twice-per-day or once-per-day LMWH dosing for the treatment of acute VTE and initial outpatient therapy over hospital admission with low-risk acute VTE, as well as against routine anti-factor Xa (FXa) monitoring to guide dosing with LMWH for VTE treatment. There was a strong recommendation (low certainty in evidence) for antepartum anticoagulant prophylaxis with a history of unprovoked or hormonally associated VTE and a conditional recommendation against antepartum anticoagulant prophylaxis with prior VTE associated with a resolved nonhormonal provoking risk factor.

2. Obstet Med. 2017 Jun;10(2):61-66. doi: 10.1177/1753495X17695696. Epub 2017

Mar 8.

'To test or not to test', the arguments for and against thrombophilia testing in obstetrics.

Ormesher L(1)(2), Simcox LE(1)(2), Tower C(1)(2), Greer IA(3).

Clinicians increasingly investigate women for thrombophilias due to their associations with venous thromboembolism and placenta-mediated pregnancy complication. These associations, however, are modest and based largely on retrospective data from studies with heterogeneous classifications and populations, leading to discordance between evidence and guidelines. Current evidence suggests a contributory rather than causative role for thrombophilia in placenta-mediated pregnancy complication and venous thromboembolism. With little evidence of benefit from antithrombotic therapy in placenta-mediated pregnancy complication, thrombophilia screening remains controversial. Given the low absolute risk of placenta-mediated pregnancy complication and gestational venous thromboembolism with heritable thrombophilia, universal screening is inappropriate. Selective screening for antiphospholipid syndrome is supported by robust evidence of benefit. Conversely, selective screening for heritable thrombophilia has not been shown to effectively manage placenta-mediated pregnancy complication. Therefore, at present heritable thrombophilia screening is not warranted for placenta-mediated pregnancy complication. Until we have better evidence from better stratified patient groups, caution should remain if we wish to practice evidence-based medicine.

3. Thromb Res. 2017 Mar;151 Suppl 1:S65-S69. doi: 10.1016/S0049-3848(17)30071-3.

LMWH in IVF - Biomarkers and benefits.

Fishel S(1), Baker DJ(2), Greer IA(3).

There is biological plausibility that coagulation activation underlies a proportion of in vitro fertilisation IVF failures and recurrent early clinical pregnancy loss (RPL). However, low-molecular-weight heparin (LMWH) use, based upon previous clinical outcome alone, is not effective in preventing RPL. RPL is heterogeneous in mechanism. Identifying those with an underlying thrombotic mechanism would allow stratification for LMWH treatment. Annexin A5 is an anticoagulant protein expressed on the trophoblast surface. The annexin A5 M2 haplotype (ANXA5 M2) is associated with several placenta mediated pregnancy complications (PMPC) and poor IVF outcome. It is transmitted equally by males and females. A pragmatic observational study of IVF couples screened for M2 carriage and treated with LMWH achieved a 37.9% live birth rate, similar to an unscreened and untreated group with fewer adverse risk factors for conception and a better prognosis from assisted conception. This suggests that LMWH may counteract the adverse effects of M2 carriage. Using this biomarker to stratify IVF and PMPC patients for LMWH treatment merits further evaluation.

4. Womens Health (Lond). 2016 Jul;12(4):433-41. doi: 10.1177/1745505716653702.

Management of inherited thrombophilia in pregnancy.

Ormesher L(1), Simcox L(2), Tower C(2), Greer IA(3).

Author information: (1)Department of Obstetrics, St Mary's Hospital, Central Manchester University Hospitals NHS Foundation Trust, Manchester, UK Maternal and Fetal Health Research Centre, Institute of Human Development, University of Manchester, Manchester, UK (2)Department of Obstetrics, St Mary's Hospital, Central Manchester University Hospitals NHS Foundation Trust, Manchester, UK Maternal and Fetal Health Research Centre, Institute of Human Development, University of Manchester, Manchester, UK. (3)Faculty of Medical and Human Sciences, University of Manchester, Manchester, UK.

Adverse pregnancy outcomes, such as pregnancy loss and pre-eclampsia, are associated with thrombotic mechanisms and thrombophilia. Antithrombotic interventions, particularly low-molecular-weight heparin, have been investigated in women identified by previous pregnancy outcome; however, the results have been inconsistent. This may reflect heterogeneity of both the study groups and the disease processes resulting in inadequate stratification to guide antithrombotic interventions. Furthermore, the variation in gestation at initiation of low-molecular-weight heparin treatment might be important. Despite limited evidence of efficacy, low-molecular-weight heparin is often used in an attempt to prevent these complications, owing to the lack of other effective treatments and its perceived safety in pregnancy. Research is required to better understand the disease processes, identify possible biomarkers and thereby more homogeneous groups for targeted treatment.

5. Blood. 2016 Nov 10;128(19):2343-2349. doi: 10.1182/blood-2016-03-703728. Epub 2016 Sep 9.

Hereditary risk factors for thrombophilia and probability of venous thromboembolism during pregnancy and the puerperium.

Gerhardt A(1)(2), Scharf RE(2), Greer IA(3), Zotz RB(2)(4).

Venous thromboembolism (VTE) is a leading cause of maternal mortality. Few studies have evaluated the individual risk of gestational VTE associated with heritable thrombophilia, and current recommendations for antenatal thromboprophylaxis in women with severe thrombophilia such as homozygous factor V Leiden mutation (FVL) depend on a positive family history of VTE. To better stratify thromboprophylaxis in pregnancy, we aimed to estimate the individual probability (absolute risk) of gestational VTE associated with thrombophilia and to see whether these risk factors are independent of a family history of VTE in first-degree relatives. We studied 243 women with the first VTE during pregnancy and the puerperium and 243 age-matched normal women. Baseline incidence of VTE of 1:483 pregnancies in women ≥35 years and 1:741 deliveries in women <35 years was assumed, according to a recent population-based study. In women ≥35 years (<35 years), the individual probability of gestational VTE was as follows: 0.7% (0.5%) for heterozygous FVL; 3.4% (2.2%) for homozygous FVL; 0.6% (0.4%) for heterozygous prothrombin G20210A; 8.2% (5.5%) for compound heterozygotes for FVL and prothrombin G20210A; 9.0% (6.1%) for antithrombin deficiency; 1.1% (0.7%) for protein C deficiency; and 1.0% (0.7%) for protein S deficiency. These results were independent of a positive family history of VTE. We provide evidence that unselected women with these thrombophilias have an increased risk of gestational VTE independent of a positive family

history of VTE. In contrast to current guidelines, these data suggest that women with high-risk thrombophilia should be considered for antenatal thromboprophylaxis regardless of family history of VTE.

6. EBioMedicine. 2016 Aug;10:298-304. doi: 10.1016/j.ebiom.2016.06.024. Epub 2016 Jul 18.

Precision Medicine in Assisted Conception: A Multicenter Observational Treatment Cohort Study of the Annexin A5 M2 Haplotype as a Biomarker for Antithrombotic Treatment to Improve Pregnancy Outcome.

Fishel S(1), Baker D(2), Elson J(1), Ragunath M(3), Atkinson G(4), Shaker A(5), Omar A(6), Kazem R(7), Beccles A(1), Greer IA(8).

BACKGROUND: Pregnancy failure and placenta mediated pregnancy complications affect >25% of pregnancies. Although there is biological plausibility for a procoagulant mechanism underlying some of these events, antithrombotic intervention trials demonstrate limited benefit, possibly through lack of stratification in heterogeneous patient groups. The ANXA5 M2 haplotype is a possible procoagulant biomarker and was tested pragmatically to determine whether this screening and LMWH treatment normalized the outcome for ANXA5 M2 positive couples. This was a pragmatic study that aimed to measure the effectiveness of a testing (for the M2 haplotype) and treatment (LMWH) pathway in routine clinical practice where there is variation between patients. Such a study in couples with fertility problems can inform choices between treatments; it is then the management protocol which is the subject of the investigation, not the individual treatments. METHODS: Couples (N=77) with one or both partners ANXA5 M2 positive demonstrated association of this haplotype with adverse IVF outcome. A pragmatic, multicenter, prospective cohort study of ANXA5 M2 haplotype screening, and LWMH treatment following embryo transfer (ET) in 103 IVF couples positive for ANXA5 M2 was performed. They were compared with a group of 1000 contemporaneous randomly selected unscreened and untreated couples undergoing assisted conception, from which 103 matched control couples were derived. The primary outcome measure was live birth incidence. Secondary outcomes were results following embryo transfer (ET) and live birth outcome by gender and M2 carriage, and allelic dose influence. FINDINGS: The tested and treated cohort of ANXA5 M2 carriers achieved a similar live birth rate (37.9%) per ET cycle compared to both the more fertile comparison group (38.5%), and to the 103 matched controls (33.0%). Significantly more treated male carrier only couples had a live birth versus female M2 only (47.7% vs. 25.0% p=0.045). INTERPRETATION: Pragmatic ANXA5 M5 screening and treatment with LMWH in couples undergoing IVF is associated with similar outcome to couples with more favorable prognostic factors. The difference in live birth outcome for treated male only carrier couples may be consistent with an additional maternal thrombophilic factor that may adversely affect pregnancy, although other mechanisms are possible. This study suggests that LMWH treatment should be started prior to clinical pregnancy.

7. Breathe (Sheff). 2015 Dec;11(4):282-9. doi: 10.1183/20734735.008815.

Pulmonary thrombo-embolism in pregnancy: diagnosis and management.
Simcox LE(1), Ormesher L(2), Tower C(1), Greer IA(3).

Author information: (1)Maternal and Fetal Health Research Centre, Institute of Human Development, University of Manchester, Manchester, UK; St. Mary's Hospital, Central Manchester University Hospitals NHS Foundation Trust, Manchester Academic Health Science Centre, Manchester, UK. (2)St. Mary's Hospital, Central Manchester University Hospitals NHS Foundation Trust, Manchester Academic Health Science Centre, Manchester, UK. (3)University of Manchester, Manchester, UK.

KEY POINTS: Venous thromboembolism (VTE) in pregnancy remains a leading cause of direct maternal mortality in the developed world and identifiable risk factors are increasing in incidence.VTE is approximately 10-times more common in the pregnant population (compared with non-pregnant women) with an incidence of 1 in 1000 and the highest risk in the postnatal period.If pulmonary imaging is required, ventilation perfusion scanning is usually the preferred initial test to detect pulmonary embolism within pregnancy. Treatment should be commenced on clinical suspicion and not be withheld until an objective diagnosis is obtained.The mainstay of treatment for pulmonary thromboembolism in pregnancy is anticoagulation with low molecular weight heparin for a minimum of 3 months in total duration and until at least 6 weeks postnatal. Low molecular weight heparin is safe, effective and has a low associated bleeding risk. EDUCATIONAL AIMS: To inform readers about the current guidance for diagnosis and management of pulmonary thromboembolism in pregnancy.To highlight the risks of venous thromboembolism during pregnancy.To introduce the issues surrounding management of pulmonary thromboembolism around labour and delivery.

8. Int J Mol Sci. 2015 Nov 30;16(12):28418-28. doi: 10.3390/ijms161226104.

Thrombophilia and Pregnancy Complications.

Simcox LE(1)(2), Ormesher L(3), Tower C(4)(5), Greer IA(6).

There is a paucity of strong evidence associated with adverse pregnancy outcomes and thrombophilia in pregnancy. These problems include both early (recurrent miscarriage) and late placental vascular-mediated problems (fetal loss, pre-eclampsia, placental abruption and intra-uterine growth restriction). Due to poor quality case-control and cohort study designs, there is often an increase in the relative risk of these complications associated with thrombophilia, particularly recurrent early pregnancy loss, late fetal loss and pre-eclampsia, but the absolute risk remains very small. It appears that low-molecular weight heparin has other benefits on the placental vascular system besides its anticoagulant properties. Its use is in the context of antiphospholipid syndrome and recurrent pregnancy loss and also in women with implantation failure to improve live birth rates. There is currently no role for low-molecular weight heparin to prevent late placental-mediated complications in patients with inherited thrombophilia and this may be due to small patient numbers in the studies involved in summarising the evidence. There is potential for low-molecular weight heparin to improve pregnancy outcomes in women with prior severe vascular complications of pregnancy such as early-onset intra-uterine growth restriction and pre-eclampsia but further high quality randomised controlled trials are required to answer this question.

Properties of Innovative Pothole Patching Materials featuring High-Toughness, Low-Viscosity Nanomolecular Resin

by Jiann-Wen Woody Ju, Member EUAS

Short Biography

Professor Jiann-Wen Woody JU received his M.S. and Ph.D. degrees from the UC Berkeley. He is a senior tenured Full Professor at UCLA, and served as the Department Chair of Civil and Environmental Engineering. Prof. Ju served as an Associate Editor for the ASME Journal of Engineering Materials & Technology, and for the ASME Journal of Applied Mechanics from 1995 to 2002. He is currently the Editor-in-Chief of the International Journal of Damage Mechanics, an Associate Editor of the ASCE J. of Nanomechanics and Micromechanics, and an Editorial Board member of the Acta Mechanica. He served as the ACI 446 Committee Chair. Prof. Ju received the 1991 Presidential Young Investigator Award from NSF and White House, 1991 Alfred Rheinstein Faculty Award from Princeton Univ., 1997 ASCE Walter Huber Civil Engineering Research Award, 1998 ASME Fellow Award, 2000 ACI-James-Instruments Award in NDE, 2006 ASCE Fellow Award, 2007 USACM Fellow Award, 2008 ACI Fellow Award, 2008-2009 Invited Chair Professor from University of Paris VI and ENS Cachan (France), 2008 Publication Award of Merit from the Structural Engineers Association, 2009-2012 Chang-Jiang Scholar Chair Professor (Ministry of Education, China), 2010 IACM Fellow Award, 2010 Kwang-Hua Chair Professor (Tongji University), 2011-2013 Tongji Univ. Chair Professor, National 1000 Talents Program (Short-Term) Distinguished Chair Professor (2013-2017), Tongji University Distinguished Chair Professor (2013-present), Guangxi University Distinguished Chair Professor (2013-present), 2013 ICACM Award, and Honorary Distinguished University Professor from Southwest Jiaotong University (2015-present), 2018 ICDM-3 Lifetime Achievement Medal, 2018 EU Academy of Sciences Member, and 2020 EMI Fellow Award, etc. Prof. Ju has published more than 180 SCI-indexed scholarly journal papers. Furthermore, Prof. Ju's journal publications have been highly cited by the Web of Science; his h-index is over 45 (Google Scholar). His research interests and research projects encompass structural engineering, structural mechanics, computational mechanics, computational damage, healing and fracture mechanics, micromechanics and nanomechanics of composites, multiscale material modeling, finite elements, biomechanics, computational geomechanics and geotechnical engineering, reliability, service life predictions, durability of concrete and cementitious composites, sulfate attack problems, environmental assessment and hazard, risk analysis and management, hazard mitigation, multiphase porous flow and transport, and coupled wind-wave-bridge interactions and damage effects, etc.

A micromechanical model of elastic-damage properties of innovative pothole patching materials featuring high-toughness, low-viscosity nanomolecular resin

H. Zhang, J. Woody Ju, W. L. Zhu, and K. Y. Yuan

Intl. J. of Damage Mechanics, March 2021

Abstract

Innovative pothole patching materials reinforced with a high-toughness, low-viscosity nanomolecular resin, dicyclopentadiene (DCPD, $C_{10}H_{12}$), have been experimentally proven to be effective in repairing cracked asphalt pavements and can significantly enhance their durability and service life. In this paper, a three-dimensional micromechanical framework is proposed based on the micromechanics and continuum damage mechanics to predict the effective elastic-damage behaviors of this innovative pothole patching material under the splitting tension test (ASTM D6931). In this micromechanical model, irregular coarse aggregates are approximated and simulated by randomly allocated multi-layer-coated spherical particles in certain representative sizes. Fine aggregates, asphalt binder (PG64-10), cured DCPD (p-DCPD), and air voids are formulated into an isotropic elastic asphalt mastic matrix based on the multilevel homogenization approach. The theoretical micromechanical elastic-damage predictions are then systemically compared with properly designed laboratory experiments as well as three-dimensional finite elements numerical simulations for the innovative pothole patching materials.

Mechanical response analysis of self-healing cementitious composites with microcapsules subjected to tensile loading based on a micromechanical damage-healing model

Kaihang Han, **J. Woody Ju**, Hao Zhang, Yinghui Zhu, Tienshu Chang, Zhengyao Wang

Construction & Building Materials, v. 280, 122251, Feb. 2021

Abstract

For the past several years, research in the field of self-healing construction materials becomes a hotspot with broad application prospects. This paper mainly focuses on the self-healing cementitious composites with microcapsules. To quantitatively interpret the self-healing effect of micro-encapsulated healing agents on microcrack-induced damage, a three-dimensional evolutionary micromechanical model is established to predict the mechanical response of the cementitious composites with the microcapsules subjected to tensile loading during the damage-healing process. The evolutionary domains of microcrack growth (DMG) and the corresponding compliances at the initial, activated and repaired stages are obtained. On the basis of the proposed 3D micromechanical model of the self-healing cementitious composites with microcapsules, elaborate studies of constitutive relations and compliance are conducted to investigate the effects of various system parameters involving the healing efficiency, fracture toughness and preloading-induced damage degrees on the compliances and stress-strain relations. The results indicate that relatively significant healing efficiency, preloading-induced damage degree and the fracture toughness of polymerized healing agent with the matrix will lead to higher tensile strength and stiffness. However, based on the two different failure modes of self-healing concrete, the excessive values of healing efficiency, preloading-induced damage degree and the fracture toughness of polymerized healing agent with the matrix will not affect the tensile strength of the cementitious composites. For the sake of the desired optimal healing effect, the specific parameters of both the matrix and the microcapsules should be selected

carefully.

Interface Energy Effect on Effective Elastic Moduli of Spheroidal Particle Reinforced Nanocomposites

Yinghui Zhu and J. Woody Ju

Acta Mechanica, April 2020

Abstract

By incorporating the interface energy effect into the classical micromechanics framework, effective elastic moduli of the composite material containing randomly distributed nanosized prolate spheroidal inhomogeneities are investigated in this paper. The effect of interface energy, which is usually neglected in classical micromechanics theories, becomes important when the size of reinforcement phase in the composite enters the nanometer range. The interface energy effect is simulated by inducing the interface stress on the zero-thickness membrane interface between the matrix and the inhomogeneities. The interfacial stress discontinuity equations are formulated in accordance with the equilibrium conditions on the idealized interface, from which the interfacial strain discontinuity is solved. Subsequently, the effective elastic moduli are derived based on the classical micromechanics homogenization approaches. Comparisons are made between the effective elastic moduli under the current nanomechanical framework and under the classical micromechanical theory. The effective elastic moduli are exhibited to be dependent upon the size of the inhomogeneities and the interface properties when the interface energy effect is considered.

Science and Technology of a Multifunctional Oxide and Nanocarbon Thin Films

by Orlando Auciello, Member EUAS

Short Biography

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

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

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

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

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

• Advanced Diamond Technologies (ADT), spun-off from Argonne National Lab (top company spun-off from a DOE Laboratory in 2003 / Profitable in 2014 /sold for profit to a large company in 2019) is commercializing industrial components and systems (UNCD-coated mechanical pump seals and bearings, and water purification systems based on electrolysis with corrosion resistant electrodes based on electrically conductive B-doped UNCD-coated metal electrodes) (Auciello is co-founder, equity holder, investor, and worked closely to develop new UNCD coated industrial products for ADT).

• Original Biomedical Implants (OBI)-USA / 2013-prsent), and (OBI-Mexico / 2016-present), developing and commercializing a new generation of UNCD-based high-tech and implantable medical devices / prostheses and medical treatments based on nanotechnology. Products in advanced state of development by OBI-USA and OBI-Mexico include: i) new generation of Li-ion batteries with anodes, cathodes, membranes, and inner walls of battery cases coated with corrosion resistant UNCD coatings, enabling LIBs with ≥ 10x longer life and safer than current LIBs, for applications to defibrillators/pacemakers, cell phones, computers, battery-powered electronic devices, and electric cars; ii) Biocompatible UNCD-coated dental implants with practically no corrosion induced in current metal-based dental implants by oral fluids (Clinical trials implanting UNCD-coated DI in 10 people, in México, demonstrated the superior performance over current commercial metal DIs ; iii) UNCD-coated metal prostheses (hips, knees) with no failure due to the protective UNCD coating; iv) new retina reattachment procedure, using biocompatible super-paramagnetic nanoparticles injected inside the eye attracted by an external temporary magnet to push the retina back into place (clinical trials performed in Argentina between 2015-2106 restored full vision to two patients (2 patents granted in USA and Japan in 2016).

Auciello has published 31 books and about 550 articles in the fields described above, holds 26 patents, and

organized, chaired, and lectured at numerous national and international conferences. He was Associate Editor of Appl. Phys. Lett (2000-2019), Journal of Materials Research (2002-2010), and currently Associate Editor of the International Journal "Coatings" (2019-present), Member of Vacuum Board (1994-2010), Integrated Ferroelectrics Board (1997-2019). Editor of two book series on thin films and applications to devices (Academic Press). He was member of the Materials Research Society (MRS) Board of Directors (2000-2003), Chair of the MRS International Relations Committee 2005-2010, ***Vice President of the MRS (2012), President of the MRS (2013), and Past President of the MRS (2014).***
He has numerous Awards, including seven R&D 100 Awards, 2003 Hispanic Engineering National Achievement Award, 2006 Federation of National Laboratories Award, 2008 University of Chicago Distinguished Performance Award, and is a ***Fellow of the AAAS and MRS.***

In recent years**, Orlando Auciello** directed fundamental and applied materials science developing a transformational multifunctional oxide super-high dielectric constant nanolaminates technology applicable to the development of new generations of supercapacitors for energy storage, new generation of CMOS gates, integrated super-high-K dielectrics/diamond films for transformational diamond-based micro/nanoelectronics beyond Silicon, and implantable medical devices, as summarized in this article

Science and Technology of Giant Dielectric Constant Oxide Nanolaminates (2011-present):
Auciello's group pioneered a breakthrough in the high-K dielectric thin film field, which consisted in the development of a new material science approach based on growing $TiOx/Al_2O_3$ nanolaminates (NLs) that produced he highest dielectric constant oxide thin films known today. For 150 nm thick $TiOx/Al_2O_3$ NLs with sub-nanometer thick sublayers, few Angstrom change in sublayer thickness dramatically increases relaxation cut-off frequency by more than 3 orders of magnitude with high dielectric constant ($k \geq 1000$). This unusual phenomenon was demonstrated to be based on the two-phase Maxwell-Wagner relaxation phenomena.

W. Li, Z. Chen, R. N. Premnath, B. Kabius, and **O. Auciello**, "Controllable Giant Dielectric Constant in Al_2O_3/TiO_2 Nanolaminates", J. Appl. Phys. **110,** 024106-1-8 (2011).

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

The R&D on super-high-k dielectric $TiOx/Al_2O_3$ NLs lead to another breakthrough development of super-high-k dielectric HfO_2/ TiOx NLs, with even superior properties to those of the $TiOx/Al_2O_3$ NLs and involving the HfO_2 film currently used in every CMOS commercial micro/nano-electronic device. A description of the new HfO_2/ TiOx NLs is presented in a recent special invited review in the MRS Bulletin.

O. Auciello, G. Lee, C. Wu, Y. Chen, J. J. Alcantar-Peña, I. Mejia, and E. de Obaldia, "Super High-Dielectric Constant Oxide Films for Next-Generation Nano-Electronics and Supercapacitors for Energy Storage". MRS Bulletin vol. 45, 232-239 (2020).

Importance: The papers cited above opened the way for the new field of science and technology of multifunctional oxide nanolaminates.

The concept of $TiOx/Al_2O_3$ nanolaminates was subsequently extended by Auciello's group to investigate and develop $BiFeO_3$ (BFO)/ $SrTiO_3$ (STO)/BFO nanolaminates (BSB-NLs). By introducing the nanoscale STO layer in between two nanoscale BFO layers, the leakage current density was reduced by two orders of magnitude with respect to relatively high leakage currents of single BFO layers (from 10^{-5} A/cm^2 to 10^{-7} A/cm^2). The BSB-NL also shows very high piezoelectric response, which is ~ 5 times higher than that of the pure BFO with the same thickness. The highly strained state of the BFO layers concurrently with the chemical/crystallographic state of the interfaces between the BFO and STO layers contribute to the very high values of piezoresponse and very low leakage current observed in the BSB-NLs.

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

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

Science and Technology of Transformational Ultrananocrystalline Diamond (UNCD™) Films Coatings (1996-present):

UNCD™ Coating for Industrial Products (1996-2012). O. Auciello and two colleagues (D. M. Gruen and A. R. Krauss) started a whole new field of materials science and technologies that resulted in the development of a novel material in thin film form defined as ultrananocrystalline diamond (UNCD™), which evolved into a new field of science and technology, currently investigated by hundreds of groups worldwide, which resulted in many hundreds of papers. Auciello and his colleagues developed a unique patented plasma chemistry involving Ar (the lowest cost inert gas) and CH_4 as the source of C atoms to grow diamond films with the smallest grains demonstrated today (2-5 nm). UNCD™ films exhibit a unique combination of exceptional mechanical, tribological, physical, chemical, electronic, thermal transport, and biocompatible properties. The multifunctionalities of UNCD™ films enables a broad range of commercial applications, namely: a) UNCD™ coatings are now in commercial mechanical pump seals (marketed by Advanced Diamond Technologies (ADT)-the first company co-founded by Auciello and a colleague, making a major impact in enabling pumps in the chemical, the oil and car industries run with 20% savings in energy usage, and in UNCD™ -coated bearings for Merck-Millipore machines mixing chemicals to produce pharmaceutical drugs; b) Atomic Force Microscope UNCD™ tips now in the market provides wear-free AFM tips for much higher resolution AFM analysis as compared with wear prone Si tips (ADT became profitable in 2014 and sold for profit to a large company in 2019); c) New diamond-based MEMS/NEMS technologies to replace the current Si-based technology that is hindering the development and commercialization of MEMS and NEMS devices, due to the poor mechanical and tribological properties of Si (new RF MEMS switches, using UNCD™ as a dielectric with controlled charging have been developed and demonstrated to produce a new generation of RF communication devices, electronic radars and more); d) New UNCD™ films-based field electron emission cathodes for application to field emission displays, cold cathodes for mass spectrometer for deep space exploration and more.

UNCD™ Coating for Encapsulation of Unique Si-based Microchip Implantable in the Human Eye to Return Partial Vision to People Blinded by the Retinitis Picmentosa Condition (2000-2010): Auciello was a member of a multidisciplinary team of scientist, medical doctors, and surgeons, developing an artificial retina to restore vision to people blinded by genetically induced degeneration of retina photoreceptors (retinitis pigmentosa). Auciello developed a hermetic bioinert/biocompatible UNCD™ coating encapsulating a Si microchip implantable inside the eye as an artificial retina– the Argus II device, marketed by Second Sight in Europe and the USA, since 2011, returns partial vision to people blind by retinitis pigmentosa, and they can read letters and recognize objects again, although diffusively, via a Si microchip receiving images from a CCD camera and injecting electronic charges into the retina ganglion cells, for transmission to the brain to form images). The Argus II artificial retina device is being implanted commercially in Europe and the USA, since 2012.

O. Auciello, "Ultrananocrystalline Diamond (UNCD™) Films as Hermetic Biocompatible/Bioinert Coating for Encapsulation of Eye Implantable Microchip to Restore Partial Vision to Blind People", Ch. 2 in "Ultrananocrystalline Diamond Coatings for New Generation High-Tech and Medical Devices" book, **O. Auciello (Ed.),** Cambridge Publisher (in press, 2021)

Materials Science and Technologies Development for Transformational Implantable Medical Devices and Prostheses Coated with the Revolutionary/Best Biocompatible/Body Fluid

Corrosion Resistant UNCD™ Coating (2013-present): Auciello founded Original Biomedical Implants (OBI-USA / 2013-present) and (OBI-México / 2016-present) with Dr. J.L. Rubio (MD) (Founder and CEO of Rubio Pharma and NICDET), the latter functional in a facility of four floors with clean rooms class 1-1000, developing new generation of UNCD™ -coated implantable medical devices and prostheses, as described below:

a) Auciello is directing R&D focused on developing a new generation of UNCD™-coated metal-based prostheses (dental implants (DI), hips, knees and many others), for which the biocompatible/body fluids corrosion resistant/lowest coefficient of friction UNCD™ coating eliminates the degradation produced in current metal-based prostheses, requiring early than desired replacement. Clinical trials on UNCD-coated DI have been conducted since 2018 to present in the World Class clinic of Dr. Gilberto López-Chávez in Queretaro-México, implanting UNCD-coated commercial Ti-alloy DI in 20 people, demonstrating that UNCD™-coated DI eliminates the ~ 15% early failure (4-5 years), worldwide, of metal implants, due to chemic al corrosion by oral fluids, inducing extreme patient discomfort and extra cost for DI replacement. UNCD™ -coated DI represent a revolution in DI technology, which will be inserted in the Mexican market by 2022-2023, followed by Latin America, Europe, Asia, and finally USA.

   K. Kam, **O. Auciello,** D.G. Olmedo, D.R. Tasat, and G. López-Chávez, "Science and Technology of Biocompatible Ultrananocrystalline Diamond (UNCD™) Coatings for New Generation of Implantable Prostheses: First Application to Dental Implants and Artificial Hips*"* Ch. 5, in **"Ultrananocrystalline Diamond Coatings for New Generation High-Tech and Medical Devices" book, O. Auciello (Ed.)**, Cambridge Publisher (in press 2021).

b) Auciello and researchers and MDs colleagues, in Argentina, are developing a new treatment for retina reattachment based on injecting a solution of superparamagnetic nanoparticles inside the eye, which are attracted by a magnetic field produced by a UNCD™-coated magnet outside the eye, attracting the particles, pushing the retina back to the eye wall for laser treatment for reattachment. Clinic al trials on two patients demonstrated that this new treatment will be transformational.

   M.A. Saravia, R. Zysler, E.Jr. Lima, A. Berra, and **O. Auciello**, "Science and Technology of Novel Integrated Biocompatible Super-Paramagnetic Oxide Nanoparticles Injectable in Human Eye and External Ultrananocrystalline Diamond (UNCD™)-Coated Magnet for New Retina Reattachment Procedure", Ch. 4, in **"Ultrananocrystalline Diamond Coatings for New Generation High-Tech and Medical Devices" book, O. Auciello (Ed.)**, Cambridge Publisher (in press 2021).

c) Auciello's group recently demonstrated that UNCD surfaces support an efficient growth of stem cells, and they are now investigating the feasibility of differentiating those cells into photoreceptors to replace the dead photoreceptors in the retina of people blinded by the death of photoreceptors, and in the future differentiation into spinal cord cells to eventually restore motion to people paralyzed by trauma of those cells, brain cells, to control or eliminate brain degradation conditions, such as Parkinson decease, and improvements in many other human conditions. This research started a new field of developmental biology based on the UNCD biocompatibility.

   B. Shi and **O. Auciello**, "Science and Technology of Novel Ultrananocrystalline Diamond (UNCD™) Scaffolds for Stem Cells Growth and Differentiation for Developmental Biology and Biological Treatment of Human Medical Conditions", Ch. 6, in **"Ultrananocrystalline Diamond Coatings for New Generation High-Tech and Medical Devices" book, O. Auciello (Ed.)**, Cambridge Publisher (in press 2021).

d) Auciello and colleagues are developing a new generation of Li-ion batteries with electrodes coated with a unique electrically conductive Nitrogen atoms-grain boundaries incorporated

UNCD™ coatings (N- UNCD™), which practically eliminate Li-ion induce chemical degradation of Natural Graphite (NG) in commercial NG/Copper anodes, which degrade the capacity energy as a function of charge discharge cycles. The N- UNCD™ coating eliminates the chamical degradation of the NG and produce practically stable capacity energy vs. charge discharge cycles, and in addition control the SEI layer formation, which is responsible for potential overheating and dangerous destruction of batteries, like the explosion of LIB in a cell phone in a plane in 2016.

O. Auciello and Y. Tzeng, "New Generation of Li-ion Batteries (LIB) with Superior Lifetime and Safety Based on Novel N-Ultrananocrystalline Diamond (N-UNCD™)-Coated Components for New Generation of Defibrillators/Pacemakers and Other Battery Powered Medical Devices" Ch. 7, in **"Ultrananocrystalline Diamond Coatings for New Generation High-Tech and Medical Devices" book, O. Auciello (Ed.)**, Cambridge Publisher (in press 2021).

The Transformational UNCD™ -coated implantable medical devices and prostheses will produce a revolution in the medical device and prostheses industry worldwide (see recent reviews mentioned below).

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

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

Recent Awards to O. Auciello

2020 **Albert Nelson Marquis Lifetime Achievement Award. Highest honor extended by Marquis Who's Who World Organization to only 5% of people of all fields listed in Who's Who base.**

2019 **Best Creativity Award in Gran Final Innostar China-USA International Technology Innovation Competition to Orlando Auciello,** for revolutionary UNCD coating technology for transformational Industrial, high-tech and medical device applications, Changsha, November 8, 2019.

Top First Prize Innostar China-USA Semifinal International Technology Innovation Competition, to Orlando Auciello, for Revolutionary Ultran-anocrystalline Diamond Coating Technology for two products (biocompatible UNCD-coated metallic dental implants with orders of magnitude superior performance than current commercial metal dental implants, and for new revolutionary Li-ion battery with electrodes coated with unique electrically conductive Nitrogen doped /Li-corrosion resistant UNCD coating, enabling new generation of LIBs with ≥ 10x longer charge/discharge life and safer than current commercial LIBs), developed and marketed by Auciello's companies (Original Biomedical Implants / OBI-USA and OBI-México), (Beijing/Shenyang-China) November 3, 2019.

Named Senior Member of the IEEE Society, for outstanding contributions to science and technology of thin films and applications to new generations of industrial, high-tech, and medical devices.

First Prize, for revolutionary biocompatible ultranancrystalline diamond (UNCD™)-coated metal dental implants with superior performance to commercial metal dental implants, at 3rd Congress of Faculties and Colleges of Dentistry, AiRC 2019, Spain.

Controlled One-pot Synthesis of Nickel Single Atoms embedded in Carbon Nanotube & Graphene Supports with High Loading

by Roland De Marco, Member EUAS

Short Biography

Present Position(s): *Deputy Vice-Chancellor (Research and Innovation) at the University of the Sunshine Coast in the Office of Research and Professor of Chemistry in the Faculty of Science at the University of the Sunshine Coast since 2016 [preceded by Pro Vice-Chancellor (Research) from 2011 and 2015].*

Role Strengths: *From July 2001 to December 2010, Roland De Marco contributed significantly to leadership and management at Curtin University progressing from Head of Chemistry to Dean of Research in Science and Engineering culminating with his past position of Associate Deputy Vice-Chancellor (Research Strategy). He is presently the Deputy Vice-Chancellor (Research and Innovation) at the University of the Sunshine Coast (from January 2016) after serving as the inaugural Pro Vice-Chancellor (Research) from 2011 and 2015.*

Roland De Marco is an internationally recognized leader in the field of electrochemical sensors. His major strength is in the field of electrochemical surface and interface analysis, and he has a strong track record in the use of state-of-the-art electrochemical and surface analytical techniques in the micro- and nano-characterization of electrochemical devices.

Experience:

January 2011-December 2020: *Adjunct Professor in the Fuels and Energy Technology Institute at Curtin University*

June 2015-June 2018: *Honorary Professor of Chemistry in School of Chemistry and Molecular Biosciences at The University of Queensland.*

January-December 2010: *Associate Deputy Vice-Chancellor (Research Strategy) in the Office of Research and Development, Curtin University and Professor of Chemistry in the Department of Chemistry, Curtin University.*

July 2007-December 2009: *Dean of Research, Faculty of Science and Engineering, Curtin University and Professor of Chemistry, Department of Chemistry, Curtin University.*

July 2001-July 2007: *Professor of Chemistry and Head of Department in Chemistry at Curtin University.*

February 1995-January 2011: *Lecturer, Senior Lecturer, Associate Professor, Professor in Chemistry at Curtin University.*

March 1992-February 1995: *Lecturer in Chemistry at The University of Tasmania.*

October 1990-March 1992: *Research Scientist at CSIRO Minerals.*

Research Focus: *Major interest in the application of electrochemical sensors to environmental and clinical analysis. I am particularly interested in research leading to publications in high impact international journals, and knowledge transfer to industry and/or the government sector.*

Leadership Focus:*The pursuit of academic excellence, so as to build internationally significant and competitive research capacity across the University. My modus operandi comprises leadership by example, "hands on" assistance to the research community, facilitation of scholarly excellence through high impact grants and publications, as well as the recruitment and retention of excellent research staff.*

Major Awards and Prizes:

2008 RACI Analytical Chemistry Lloyd Smythe Medal for excellence in research, teaching and service to the chemical profession in Australia

1999 Curtin University, Centre for Educational Advancement Innovative Teaching Award

1989 Bloom-Guttmann Prize for the best presentation by a young electrochemist at the 10th

Australian Symposium on Analytical Chemistry
Publication Summary:
142 Papers in International Journals and 2 Book Chapters at H-Index of 30 and field weighted citation impact (FWCI) of 2.03 (sourced from Scopus/SciVal on 6 March 2020)

1) Zhao, Shiyong, Wang, Tianshuai, Zhou, Guanmin, Zhang, Liji, Lin, Chao, Veder, Jean-Pierre, Johannessen, Bernt, Saunders, Martin, Yin, Lichang, Liu, Chang, De Marco, Roland, Yang, Shi-Ze, Zhang, Qianfan, and Jiang, San Ping, ChemNanoMat, Vol. 6, pp. 1063-1074, 2020.

Controlled one-pot synthesis of nickel single atoms embedded in carbon nanotube and graphene supports with high loading

Abstract

Single-atom catalysts (SACs) have attracted much attentions due to the advantages of high catalysis efficiency and selectivity. However, the controllable and efficient synthesis of SACs remains a significant challenge. Herein, we report a controlled one-pot synthesis of nickel single atoms embedded on nitrogen-doped carbon nanotubes (NiSA−N−CNT) and nitrogen-doped graphene (NiSA−N−G). The formation of NiSA−N−CNT is due to the solid-to-solid rolling up mechanism during the high temperature pyrolysis at 800 °C from the stacked and layered Ni-doped g-CN, g-CN−Ni structure to a tubular CNT structure. Addition of citric acid introduces an amorphous carbon source on the layered g-CN−Ni and after annealing at the same temperature of 800 °C, instead of formation of NiSA−N−CNT, Ni single atoms embedded in planar graphene type supports, NiSA−N−G were obtained. The density functional theory (DFT) calculation indicates the introduction of amorphous carbon source substantially reduces the structure fluctuation or curvature of layered g-CN-Ni intermediate products, thus interrupting the solid-to-solid rolling process and leading to the formation of planar graphene type supports for Ni single atoms. The as-synthesized NiSA−N−G with Ni atomic loading of ∼6 wt% catalysts shows a better activity and stability for the CO reduction reaction (CORR) than NiSA−N−CNT with Ni atomic loading of ∼15 wt% due to the open and exposed Ni single atom active sites in NiSA−N−G. This study demonstrates for the first time the feasibility in the control of the microstructure of carbon supports in the synthesis of SACs.

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Deactivation and selectivity for electrochemical ozone production at Ni- and Sb-doped SnO_2 / Ti electrodes

Abstract

This work reports on a time-resolved study of the deactivation of electrochemical ozone production (EOP) active anodes using a novel approach to measure total ozone production. The reproducibility and change of the electrodes over time have been investigated using a number of electrochemical and physical techniques. The dissolution of antimony from the surface of the nickel- and antimony-doped tin oxide (NATO) electrode is the main process

behind the deactivation of the EOP. When surface antimony is depleted, the continued deactivation seems to be connected to the dissolution of nickel. Despite tin (from the coating) and titanium (from the substrate) continuously dissolving during galvanostatic polarization of the NATO electrode, our experiments point to no connection between these processes and the EOP activity. In addition, the selectivity of the electrode is affected by electrolyte penetration, accessing fresh reaction sites that are active on the EOP. The results indicate that both antimony (III) and nickel present at the surface of the NATO are responsible for the EOP activity.

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A universal seeding strategy to synthesis single atom catalysts on 2D materials for electrocatalytic applications

Abstract

Single-atom catalysts (SACs) are attracting significant attention due to their exceptional catalytic performance and stability. However, the controllable, scalable, and efficient synthesis of SACs remains a significant challenge. Herein, a new and versatile seeding approach is reported to synthesize SACs supported on different 2D materials such as graphene, boron nitride (BN), and molybdenum disulfide (MoS2). This method is demonstrated on the synthesis of Ni, Co, Fe, Cu, Ag, Pd single atoms as well as binary atoms of Ni and Cu codoped on 2D support materials with the mass loading of single atoms in the range of 2.8-7.9 wt%. In particular, the applicability of the new seeding strategy in electrocatalysis is demonstrate on nickel SACs supported on graphene oxide (SANi-GO), exhibiting excellent catalytic performance for electrochemical CO2 reduction reaction with a turnover frequency of 325.9 h(-1) at a low overpotential of 0.63 V and high selectivity of 96.5% for CO production. The facile, controllable, and scalable nature of this approach in the synthesis of SACs is expected to open new research avenues for the practical applications of SACs.

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Hydrogen release from carbon steel in chloride solution under anodic polarization

Abstract

The hydrogen permeation current increase was noticed for carbon steel in 0.5 mol/L NaCl solution under strong anodic potentials, which is contrary to the common understanding. Hydrogen permeation under cathodic potentials has been widely studied because of possible hydrogen embrittlement failures of high strength steels in seawater, but investigations of anodic polarization on hydrogen permeation are fairly rare, as the

hydrogen evolution reaction shall be retarded. To corroborate the observed phenomenon, experiments were conducted using both as-received and vacuum-annealed sheet specimens. It was verified that the observed phenomena originated from the released hydrogen in traps by metal dissolution under anodic polarization.

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Magnetizing lead-free halide double perovskites

Abstract

Spintronics holds great potential for next-generation high-speed and low–power consumption information technology. Recently, lead halide perovskites (LHPs), which have gained great success in optoelectronics, also show interesting magnetic properties. However, the spin-related properties in LHPs originate from the spin-orbit coupling of Pb, limiting further development of these materials in spintronics. Here, we demonstrate a new generation of halide perovskites, by alloying magnetic elements into optoelectronic double perovskites, which provide rich chemical and structural diversities to host different magnetic elements. In our iron-alloyed double perovskite, Cs2Ag(Bi:Fe)Br6, Fe3+ replaces Bi3+ and forms FeBr6 clusters that homogenously distribute throughout the double perovskite crystals. We observe a strong temperature-dependent magnetic response at temperatures below 30 K, which is tentatively attributed to a weak ferromagnetic or antiferromagnetic response from localized regions. We anticipate that this work will stimulate future efforts in exploring this simple yet efficient approach to develop new spintronic materials based on lead-free double perovskites.

Deeper Understanding of the Basic Organizing Principles of the Immune System

by Max D. Cooper, Member EUAS

Short Biography

Professor of Pathology and Laboratory Medicine, and Member of the Emory Vaccine Center, Emory University School of Medicine

Education-Training

Tulane University Medical School, New Orleans, LA, 06/1957, Medicine
Saginaw General Hospital, Saginaw, MI, 06/1958, General Medicine
Tulane University Medical School, New Orleans, LA, 06/1960, Pediatrics
Hospital for Sick Children, London, England, 5/1961, Pediatrics & Neurology
University of California at San Francisco, CA, 06/1962, Allergy & Immunology
University of Minnesota, Minneapolis, MN, 06/1966, Immunology Research

***Personal Statement**. I am a physician/scientist. Providing medical care for children with unusual susceptibility to infections early in my career triggered an abiding interest in learning more about normal immune system development and function in order to explore the pathogenesis of immunological disorders, immunodeficiency diseases and lymphoid malignancies in particular. This interest has fueled my sustained effort to gain a deeper understanding of the basic organizing principles of the immune system with the goal of translational application of this information.*

Positions and Employment

1962-1963 Instructor in Pediatrics, Tulane University Medical School, New Orleans, LA
1966-1967 Assistant Professor of Pediatrics, University of Minnesota, Minneapolis, MN
1967-2008 Professor of Pediatrics and Microbiology, University of Alabama at Birmingham
1971-2008 Senior Scientist, Comprehensive Cancer Center, UAB
1973-1974 Visiting Scientist, Tumor Immunology Unit, Dept. of Zoology, University College of London
1984-1985 Visiting Professor, Institute of Embryology and Pasteur Institute, Paris
1987-2008 Professor of Medicine and Director, Division of Developmental & Clinical Immunology, UAB
1988-2006 Howard Hughes Investigator, UAB, Birmingham, AL
2008-present Professor of Pathology and Laboratory Medicine, Emory Vaccine Center and Georgia Research Alliance Eminent Scholar, Emory University, Atlanta, GA

Other Recent Experience

2005-2019 Member/Chair of Scientific Advisory Board (SAB), Center for HIV/AIDS Vaccine Immunology (CHAVI), Duke University
2008-2018 Member, SAB, Max-Planck Institute of Immunobiology and Epigenetics, Freiburg, Germany
2008-2018 Member, SAB, Imagine Foundation, Paris, France
2013-2019 Member, SAB, Scripps Center for HIV/AIDS Vaccine Immunology and Immunogen Discovery
2011-present Member, Board of International Scientific Advisors, Foundation for Primary Immunodeficiency Diseases

Honors

I am an elected member of the National Academy of Sciences (1988), the National Academy of Medicine (1990), the American Academy of Arts and Sciences (1992), foreign associate member of the French Academy of Sciences (2015), Foreign Associate, Royal Society of London (2019) and EU Academy of Sciences (2020). I am a former president of the American Association of Immunologists (1988-1989), the Clinical Immunology Society (1993-1994) and the Kunkel Society

(2009-2011). Research honors include the Founder's Award of the Society for Experimental Biology and Medicine (1966), Sandoz Prize in Immunology (1990), American College of Physicians Science Award (1994), American Association of Immunologists (AAI) Lifetime Achievement Award (2000), AAI-Dana Foundation Award in Human Immunology Research (2006), Avery Landsteiner Prize (2008), the Robert Koch Prize (2010), the Japan Prize (2018) and the Albert Lasker Basic Medical Research Award (2019). Mentorship awards include the Emory University Postdoctoral Education Office One in One Hundred Mentor Award (2009) and AAI Excellence in Mentoring Award (2012).

Contributions to Science

Working with Raymond Peterson in Robert Good's laboratory at the University of Minnesota, I conducted experiments in chickens that defined two major lineages of lymphocytes: one that is derived from the thymus and mediates cellular immune functions, and the other of which is derived from the bursa of Fabricius and is responsible for producing antibodies that mediate humoral immunity.[1,2,3] These findings coupled with information obtained in contemporaneous studies of mouse models and heritable immunodeficiency diseases led directly to the understanding that two developmentally-separate, but functionally-intertwined populations of lymphocytes, called T cells and B cells, are central components of the adaptive immune system in all jawed vertebrates. Our original schematic model of T and B lymphocyte development and function provided a framework for the classification of immunodeficiency diseases and lymphoid malignancies, served as a roadmap for successful transplantation therapy of certain immunodeficiency diseases[4], and raised fundamental questions about the nature of the receptors that T cells use to see antigens, how T and B cells work together, and where B cells are generated in mammals.[5]

In my laboratory at the University of Alabama at Birmingham, my colleagues and I found that B cells with IgM receptors can switch to the production of other antibody classes[6,7]; these studies also revealed that ligation of the IgM receptors on immature B cells induced cell death or aborted cellular differentiation. Our search for the site(s) in which mammalian B cells are produced eventually led to the demonstration, with John Owen and Martin Raff at University College London, that mouse B cells are generated in hematopoietic tissues, primarily the fetal liver and bone marrow[8,9]. The composite results obtained in this series of studies enabled us to identify the precursors of mammalian B cells.

After validating and refining our early model of mammalian B cell development in studies of humans[10], we used this information to determine the developmental stages at which B cell differentiation is aborted in antibody deficient patients[11,12] or arrested in B lineage malignances, to wit the pro-B or pre-B status of childhood acute lymphocytic leukemia versus later stage B cell malignances, such as B cell leukemia, B cell lymphomas and multiple myeloma[13-15]. These early findings contributed to the definition and, ultimately, to the development of better treatment options for these diseases.

In studies of avian T cell development, we found that *TCR* gene excision circles (TREC) are present in recent T cell emigrants from the thymus and that their assessment can be used to monitor thymus function[17]. The original findings in chickens were validated in mice[17], and the TREC assay adapted for use in humans by Daniel Douek and others provided an invaluable non-invasive test for thymic function.

More recently, my colleagues and I have discovered an alternative adaptive immune system in lampreys and hagfish, the extant jawless vertebrates that last shared a common ancestor ~480 million years ago. In their alternative adaptive immune system, leucine-rich-repeat gene segments are used instead of immunoglobulin gene segments to generate a vast repertoire of variable lymphocyte receptors (VLR) for antigen recognition[18]. Equally surprising, we found that the *VLRA*, *VLRB* and *VLRC* genes are assembled by separate lineages of lymphocytes resembling the T and B lymphocytes in jawed vertebrates[19,20]. Our findings have redefined the current view of how an adaptive immune system evolved. They indicate that the dual nature of lymphocyte development and function is a fundamental design feature of the adaptive immune system in both jawless and jawed vertebrates, and reveal the convergent evolution of alternative mechanisms for generating specific antigen receptors. The unique structure and novel specificities of lamprey VLR antibodies further attest an important translational potential for biomedical purposes[21,22].

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Covid 19 is the Game Changer for Healthcare Transformation and the Breakthrough of Health Technology

by Pascal Verdonck, Member EUAS

Short Biography

Pascal Verdonck was born in 1963 in Gent, Belgium. He graduated as Master of Science Civil Engineering in 1986 from the Ghent University. He obtained his diplomas in Master of Business Administration (1989), Master of Science Biomedical Engineering (1993) and PhD (1993) from the Ghent University. He is married with Nathalie Van Peteghem and has two children Simon (°1993) and Charlotte (°1995)

Professional activities and relevant experience

- *Assistant (1987-1992), post-doctoral researcher (1993-1995), assistant professor (1996-2002) and full professor "cardiovascular mechanics and biofluid dynamics "at the Ghent University since 2002*
- *Visiting professor University of Groningen, Groningen , the Netherlands (2001-2007)*
- *Visiting professor Imperial College, Londen (2004-2008)*
- *Tenured professor at the International Faculty for Artificial Organs, Bologna, Italy*
- *Head of the Department of Civil Engineering of the Ghent University (1998-2006)*
- *Ombudsman of the Faculty of Applied Sciences of the Ghent University (1993-2003)*
- *Chairman bachelor programs of the Faculty of Applied Sciences of the Ghent University (2003-2006)*
- *Scientific secretary of the Institute Biomedical Technology of the Ghent University (1997-2006)*
- *Visiting professor University Paris XII (1997)*
- *Visiting Socrates professor TU Kosice (2000-2004) and Julich (2000-2010)*
- *Member Board European Society for Engineering and Medicine (2002-2004)*
- *Member of the Board of Trustees of the International Society for Artificial Organs ISAO (1999-2003)*
- *Member of the Board of the ESAO European Society for Artificial Organs (2004-2011)*
- *Vice Chairman of the alumni of the engineers studied at the Ghent University (1995-2003)*
- *Vice Président "Société Biomécanique" (2000-2002) , Président "Société Biomécanique" (2002-2004)*
- *Member evaluation commission Belgium for " medical devices" and "active medical devices " (2001-2007)*
- *Chairman of the Board of Directors start-up "FluidDA" (2007- 2009)*
- *Member of the Board of Directors AZ Maria Middelares hospital Gent (2000-2007)*
- *CEO of private hospital "AZ Maria Middelares" Gent (2007- 2015) (www.azmmsj.be)*
- *Senior full professor "MedicalTechnology" Ghent University (2007-) (www.ugent.be)*
- *Visiting Professor "biomedical engineering" Catholic University Leuven, Belgium (2009-)*
- *Chairman National Committee Biomedical Engineering (2001-) (www.ncbme.be)*
- *Member of the Royal Flemisch Academy of Belgium for sciences and arts (2009-)*
- *Member of the Board of Directors OLV Aalst Hospital (2012-) (www.olvz.be)*
- *Member of the Board of Directors Acerta (2013) (www.acerta.be)*
- *Vice chairman of the Board of Directors Artevelde University College Gent (2005-) (www.arteveldehs.be)*
- *Vice Chairman Belgian Association Hospital Directors (2013-) (www.ziekenhuisdirecteurs.be)*
- *Member of the Board of Directors Voka Flanders chamber of commerce and industry (2015-)*
- *Chairman of the Board of Directors AZ Maria Middelares hospital Gent (2015-) (www.azmmsj.be)*

- *CEO MedTech Flanders (www.medtech.flanders.be) (2015-)*
- *Member of the board of Directors Sint-Vincentius Deinze Hospital ((2017-)*
- *Member of the board of Directors Jan Yperman Hospital Ieper ((2019-)*
- *Board Member European Association Hospital Managers (2019-) (www.eahm.eu.org)*

Actual academic courses

- *"Biosystems", 2nd year bachelor engineering sciences @Ghent University*
- *"BioFluid Mechanics", 2nd year master biomedical engineering sciences @Leuven University*
- *"Leadership in Healthcare", 2nd year master biomedical engineering sciences @Ghent University*
- *"Engineering project in a hospital", 2nd year master biomedical engineering sciences @Ghent University*

Research and innovation

His scientific research has spanned numerous fields of biomedical engineering sciences : experimental and numerical modeling of the cardiovascular system, haemodynamics and transport phenomena in extracorporeal circulation and artificial organs, computational biodesign and medical device technology. He is an active advisor for the MedTech Start & Scale-up Ecosystem.

MedTech is the driver towards a more Sustainable Healthcare

Health is a state of complete physical, mental and social well-being. Healthcare is thus only a minor component for the health of an individual. In 2010, the European Commission defined the primary goal of healthcare policy as that of maximizing the health of the population within the limits of the available resources, and within an ethical framework built on "equity and solidarity principles". This goal encompasses three pillars of major importance: maximize health, with limited resources, in an ethical framework. Over the last decade the goal to maximize health has not changed, however the limitations and the framework surrounding this goal have changed significantly including the call for more social responsibility and sustainability, the fear of the impact of climate change and Covid 19,…

Achieving this original ambition in a sustainable manner requires strong leadership and everything starts with the vision from a patient focus. It is medical technology (MedTech) with medical devices ranging from preventive diagnostic in vitro test, to digital applications that drives this digital transformation towards a value-based, connected and finally to integrated care around a patient.

Covid 19 is the Game Changer for Healthcare Transformation and the Breakthrough of Health Technology

Covid-19 has changed the world. The fight against the COVID is not won with a vaccine in sight. We are still all adapting our way of living ("on line" customer & retail service), our way of working, way of care provision & cure by accelerating new ((bio)engineering & technology. "Necessity is the mother of invention" said Plato and so we feel nowadays the fourth industrial revolution: the acceleration towards a bio-revolution (biopharma, biomolecules, biosystems, biomachines, bioengineering, biocomputing,..). In healthcare we became open for a new generation of "health conscious" consumers & "tech-fan" healthcare providers.

Health technology (Health Tech), is defined according the World health Organisation as "application of organized knowledge and skills in the form of devices, medicines, vaccines, procedures and systems developed to solve a health problem and improve quality of lives". In our opinion it can be classified in three categories: Biotech, Digital Health and MedTech:

1. (Red) BioTech, is the use of living systems (cells, biomolecular processes) to develop technologies and products to help and heal people
2. Digital Health means the use of information and communication technologies to help address the health problems and challenges faced by patients. The European Patient Forum defines it as health care practices supported by electronic processes & communication
3. Medical technology including:
    - Medical devices including surgical tools, implants, active devices and active implantable technology
    - In-vitro diagnostics including self-test, bedside and laboratory equipment
    - Embedded or stand-alone software

Within health technology, the MedTech is subject to strict European quality and safety rules (EU Medical Device Regulation). However, its use often still depends on the experience of the healthcare provider, the quality of the hospital and the knowledge of the user.

A three shift Model in our Society

This parallel evolution for striving to more sustainability & social responsibility, the tsunami of introducing new (medical) technology and the pandemic, and according economic and mental crisis are leading to three fundamental shifts.

The first shift goes beyond the concept of *hospital to the concept of community*. This allows patients to receive good and appropriate care within their own community and thus closer to home. This does not mean that the hospitals become redundant, but that they organize care close to or in the comfort of the patients' home. This could include telemedicine, chronic care management, patient remote monitoring, patient self-management with or without coaching, etc. This is not only more comfortable for the patient and more affordable for the system, it is also essential in areas where people do not have easy access to advanced medicine and hospital care.

The second shift is *from healthcare to health*, meaning caregivers would not simply act in the healthcare process but in fact intervene in the prevention and pre-care process to enable better and healthier living conditions for their previous, current and future patients. This health continuum describes how clinicians should not only focus on diagnosis and treatment but also get involved across the patient care spectrum, in healthier living, prevention and home care. This starts from the idea that citizens are in a continuous loop. When citizens are treated and receive home care, they are treated as patients. Once they are fully recovered, they go back to being citizens. However, chances are high that if no change in their way of life is initiated, they will quickly return to being patients in the diagnosis phase. As citizens are either future or past patients, it is logical that healthcare practitioners are connected to both citizens and patients.

The third shift is to go from *quality to value*, and to offer every patient the best possible value he or she can get. Quality means that the delivered care is safe (that does not harm patients), effective, (consistent with best professional knowledge), patient-centered and meets the needs of the patients. This revolution towards value i.e quality over cost will be discussed in the next paragraph.

Towards value-based connected and integrated care

Within these frameworks, three healthcare concepts play an important role: value-based, connected and integrated healthcare. All three are interconnected.
The idea of *value-based healthcare* is that the goal and purpose of healthcare in general is to improve the value for patients. Value is the product of the patient's personal experience with his or her outcome divided by the cost to achieve this outcome.
Value= (patient' s experience*patient' s outcome)/(cost to achieve patient' s outcome)

But this definition means also value for the caregivers, the health system, the relatives of the patient,… As M. E. Porter said, the only way to unite the interests of all participants in the healthcare ecosystem is by using value as a goal. Value is created by caring for a patient's medical condition over the full cycle of care. The improvement of the outcomes are the most powerful single lever in order to reduce costs and improve value.

The second concept is *integrated care*. Integrated care brings together inputs, delivery, management and organisation of services related to diagnosis, treatment, care, rehabilitation and health promotion. Nowadays, a hospital or an individual healthcare professional can no longer operate in isolation. All of these individuals are integrated into one or more healthcare networks. Once a patient consults a healthcare worker of a certain network, he or she automatically becomes part of this network, of course with the liberty to leave or change as it pleases.

The last concept is *connected care*. We are increasingly confronted with smart environments. Wearables, smart cameras, ambient technology, connected equipment, etc. are embedded in a world where the Internet of (medical) Things is growing exponentially and everything and everyone is becoming connected. This connection can be seen at different scales, going from on-body to in-home to community, in-clinic or in-hospital settings. When a patient is treated with a certain device or undergoes a certain examination, digital data will be generated, stored and used by other devices, people, institutions or environments in order to improve the value for the patient.

Towards a health data framework turning data into value

Value, integration and connection are based on data. Without data that measures a patient's outcomes and costs, the value to optimize the healthcare process cannot be calculated. Without efficient data exchange, healthcare networks described above cannot operate and healthcare staff would once again work on their own isolated islands, leading to redundant examinations and consultations.

The healthcare of the future will generate massive volumes of data. Connected devices, healthcare workers and patients will create and use data lakes. Sensors will perform the data collection from health, activity, location, emotions, parameters, etc. They will be the well of the data lake. One should not only think of wearables or insideables that monitor parameters of the patient but also the external ambient sensors that measure humidity, temperature, weather, pollution, etc. Measuring the living environment of a patient is something that is already done with a technique called ambient intelligence. Ambient intelligence creates a digital environment that is aware of the individual's presence and context, and is sensitive, adaptive, and responsive to their needs, habits, gestures and emotions. Combining these measurements with the patient-specific data allows for a more patient-specific approach. This data, used as currency in the network, can take many forms, ranging from personal to population or environmental data and will be transferred between a variety of interested parties. It is "data science" that forms the important connection with

the above ambition of a value based, connected and integrated care and the future of digital therapy as part of e-health, m-health and telemedicine.

Big Data can be definied the capacity to search, aggregate and cross-reference large data sets. The “Big Data” ecosystem consists of five components: (1) data creation, (2) data collection and management, analysis and information extraction, (3) hypothesis and experiment and (4) decision-making and action. So “Big Data” is undeniably a process, let’s call it data science. The “Big Data” ecosystem includes the application of advanced heuristics, statistical procedures, neural networks, machine learning algorithms, artificial intelligence techniques, ontology based search strategies, inductive reasoning algorithms, pattern recognition, prediction algorithms,… with the aim of arriving at meaningful characteristics and patterns. Two key bottlenecks are still not completely solved for healthcare data: improving data quality & enriching available data. Hospitals with good data available for analysis are attractive partners for all kinds of research projects like "discovery science" (in-depth understanding of the development of a disease), in "clinical development" (use of data to improve the efficiency of clinical studies), "post-authorization obligations ”(continuous monitoring of patients on certain medications),…
Nowadays, data is typically spread over different entities: central servers of hospitals, decentralized personal different communication protocols can establish a connectivity (data transmission) between all those different parties in this integrated and connected care network: Wi-Fi, Bluetooth, cellular (3G, 4G, 5G), LoRa, etc. Of course, merely collecting and transporting data will not be enough. This continuous flow of data collection will outgrow the storage capabilities of modern-day healthcare infrastructures, and the IoMT and decentralized healthcare will only increase further the demand for storage space.
Physical examinations will be partly substituted by a flow of digital information. Such a huge volume of data could easily overwhelm healthcare workers, leading to a situation in which value and patient outcomes no longer improve. The amount of non-processed data might lead to a decrease in efficiency and poor use of time, and thus also to a worsening of patient outcomes.

Therefore, next to collection, currency and transmission, intelligence needs to be introduced into the data framework. This intelligence, when done by computers is called artificial intelligence (AI) and can be a great asset to healthcare teams. AI is able to analyze data in order to provide insights that can inform the actions of healthcare staff, decision-makers or the patients themselves. Signals that would otherwise go unnoticed or reacted upon too late can now be detected by the AI to trigger alarms directly to the responsible party. The use of this artificial intelligence in healthcare can be put into three categories: knowledge-based decision support systems, data-driven clinical decision support systems and computer-aided diagnosis.

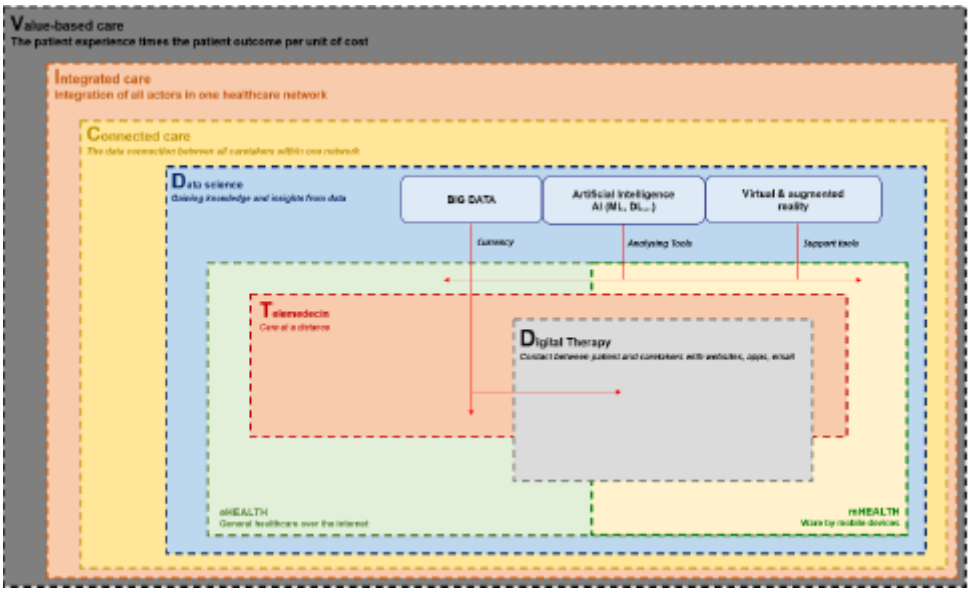
Last but not least, an important aspect of data is security. With the new GDPR regulations of 2018, data protection has gained a tremendous importance over the last two years. This, in combination with a huge volume of generated data, leads to the necessity of rethinking the concept of data protection as a whole.

The possibility to use this data in a secured and effective way will lead to an increase of the future value of health care. So future value will be equal to innovation to the power of data. Hence, without data, innovation will not create any value or vice versa.

Impact of medical technology towards sustainable healthcare

The above explained evolution can be in my opinion summarized in one key figure. The vison is based an evolution towards value-based, integrated and connected care where data

science (including big data, artificial intelligence and augmented & virtual reality) is the hinge between the patient centric approach and e-health, m-health, telemedicine towards digital diagnosis and therapy.



Conclusion

Achieving the original ambition to maximize health, with limited resources, in an ethical framework in a sustainable manner requires patient focus. This means that healthcare is transformed, step by step to a value based, connect healthcare leading finally towards integrated care around an individual. It is medical technology (MedTech) that drives this digital transformation connecting data science with digital diagnosis & therapy. Thanks to sensors, data & algorithms.

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U Identification of Glutathione within Neuronal Cells

by George Perry, Member EUAS

Short Biography

George Perry is Professor of Biology and Chemistry, Semmes Foundation Distinguished University Chair in Neurobiology, and former Dean of Sciences at The University of Texas at San Antonio. Perry has studied Alzheimer's disease since 1982 and was the first to discover that oxidative stress is a key feature of this and related neurodegenerative diseases. His studies identified oxidative damage, its source from metabolic/mitochondria failure and catalysis by iron and copper. This work led to a novel interpretation of the role of amyloid—that instead of causing Alzheimer's disease, it is a protective antioxidant response, and the reason all the amyloid-based therapies have failed.

Perry received his Bachelor of Arts degree in zoology with high honors from University of California, Santa Barbara. After graduation, he headed to Scripps Institution of Oceanography and obtained his Ph.D. in marine biology under David Epel in 1979. He then received a postdoctoral fellowship in the Department of Cell Biology in the laboratories of Drs. Bill Brinkley, Anthony Means and Joseph Bryan at Baylor College of Medicine where he laid the foundation for his observations of abnormalities in cell structures.

He is distinguished as one of the top Alzheimer's disease researchers with over 1000 publications, one of the top 100 most-cited scientists in neuroscience and behavior and one of the top 25 scientists in free radical research.

Perry has been cited over 92,000 times and is recognized as an ISI highly cited researcher (H=153). Perry is editor-in-chief for the Journal of Alzheimer's Disease, the most cited journal in the field. He is a fellow of the American Association for the Advancement of Sciences, Texas Academy of Sciences, and the Microscopy Society of America. He is past-president of the Southwestern and Rocky Mountain Division of the American Association for the Advancement of Science and past-president of the American Association of Neuropathologists. He was awarded the Society for the Advancement of Chicanos and Native American in the Sciences' (SACNAS) Distinguished Professional Mentor Award, the Senior Investigator Award of the International College of Geriatric Psychoneuropharmacology (ICGP), Martin Goland Award of the Alamo Chapter of Sigma Xi, and Senior Fulbright Scholar. He was elected a Foreign Corresponding Member of the Academy of Sciences of Lisbon, Foreign Correspondent Member of the Spanish Royal Academy of Sciences, Corresponding Member of the Mexican Academy of Sciences, and Member of the Dana Alliance for Brain Initiatives.

For over a decade, Perry hosted the Texas Science and Engineering Fair. He has mentored over a hundred students and fellows in research.

U Identification of Glutathione within Neuronal cells

Texas Academy of Science 123rd Annual Meeting, p.50, 2020

Diego Rojas, Abstract Submission; George Perry, Co-Author

In Alzheimer's disease (AD), there is a misconception regarding the fate of neurons undergoing oxidative stress(OS). Two common stances prevail, one supporting the pathway favoring the death of neurons or alternatively that neurons avoid at all costs cell death in order to preserve vital neurochemical connections. In this study, we analyzed glutathione (GSH), arguably the most important cellular antioxidant critical to neuronal survival, and free sulfhydryls in the pathology of oxidative stress and cell death in AD. This pinpointed how neurons persist in AD through years of chronic OS and apoptosis entry. This being likely to indicate the pentose phosphate pathway (PPP) is critical to protecting the neurons from death through GSH production. The research conducted observed the behavior of neurons and the presence of GSH within brain tissue through various anti-glutathione antibodies utilized in tissue staining. In conclusion, this experiment utilized anti-glutathione antibodies to note if GSH accumulates in AD through the various stages of AD progression, allowing for a clearer understanding of neurons in regards to PPP radicals and OS in conjunction with future development of drugs focused around the PPP and increases in GSH.

A101 Mass Spectrometry Imaging of Alzheimer's Disease Tissue - Plaques and Colocalization Madeline E. Colley, Andrea R. Kelley, Stephan B.H. Bach, Xiongwei Zhu, and Geoge E. Perry The University of Texas at San Antonio, San Antonio, TX; Case Western Reserve University, Cleveland, OH Introduction: Mass spectrometry imaging (MSI) is a technique that allows for the visualization of hundreds species on tissue sections. Brain banks often contain ethanol-fixed (EF) tissues which do not crosslink proteins but maintains tissue morphology and rigidity. The novel method described is designed to streamline the sample preparation process while optimizing molecular species of AD brain tissue relating to plaque moieties. We demonstrate the method to visualize plaques and lipids in EF and fresh-frozen AD brain tissue as well as co-localize lipid species to amyloid-beta peptide clips indicative of senile plaques. Methods: Archived, paraffinembedded tissue blocks and fresh-frozen hippocampus brain were supplied by the Case Western Reserve University Brain Bank. Fresh frozen tissue was embedded in gelatin and carboxymethyl cellulose. Tissue was sectioned onto indium-tin oxide (ITO) slides at 8

μm thickness. Sections were placed on conductive, grapheneoxide tape for MALDI analysis. A Bruker UltrafleXtreme MALDI-TOF/TOF mass spectrometer was used for MSI. 500 shots were acquired per pixel with 100 μm spatial resolution. Results: EF tissues preserves lipid species moreso than formalin-fixed. Wax removal with xylenes also removes lipids, so our method keeps the lipids intact. There is good agreement between fresh-frozen and ethanol-fixed tissue which ensures that 65 archival tissues can indeed be used to visualize lipids in AD brain tissue. We developed a method which allows for the direct visualization of amyloid-beta 1-40 and 1-42 in ethanol-fixed tissues. To further confirm our identifications, we used spatial shrunken clustering on the MSI data sets to separate the signals of the plaques from the other proteins. We used the ethanol-fixed hippocampus tissues from two separate AD patients to confirm the validity of our method. Experiments with fresh-frozen tissue have shown that ceramide and phospholipid species are colocalized with the amyloid-beta plaques. Conclusions: We demonstrate the usefulness of ethanol-fixed tissue for visualizing intact proteins and lipids in human AD brain tissue. This is a novel way to visualize senile plaques in AD tissue. Furthermore, the use of the graphene tape in the lipid imaging allowed for removal of wax without removing lipids in the ethanol-fixed tissue. In addition, we utilized fresh-frozen tissue to confirm the ethanol-fixed identifications as well as provide colocalization data between lipid and protein species.

Formalin-based vs. alcohol-based fixatives for mass spectrometry imaging of Alzheimer's disease tissue

Savannah Dyer, Andrea Renee Kelley, Madeline Colley, Stephan Bach, Xiongwei Zhu, George Perry, Stephan B.H. Bach

Introduction

Mass spectrometry imaging (MSI) is able to provide spatial and morphological information for a variety of analytes including, proteins, peptides, and lipids. Tissues utilized for this type of analysis are routinely fixed, in order to preserve native structures, and paraffin-embedded. Fixatives range from formalin-based, which cross-links proteins, to alcohol-based, which dehydrates the tissue and coagulates proteins. There are significant challenges to overcome when utilizing cross-linked tissue for MSI due to the inability to reproducibly relax cross-links and enzymatically produce peptide fragments sufficient for analyte identification. Here, we compare the applicability of several tissue fixatives (ethanol and formalin) in the MSI analysis of hippocampal tissue from Alzheimer's disease (AD) and control human brain tissue. Cardinal R Studio was utilized in an attempt to identify unknown proteins within the ethanol fixed paraffin embedded tissues.

Methods

AD and control archived brain tissue was provided by Case Western Reserve University. All tissue blocks were embedded in paraffin and fixed in various solvents (ethanol and formalin) prior to reciept. Serial sections were cut at 10 μm and mounted onto ITO-conductive glass slides for MSI and glass microscope slides for hydrogel experiments. All samples underwent the same preparation procedure including deparaffination and

washing to remove salts and lipids. Tissue fixed with cross-link inducing fixatives underwent additional preparation to relax cross-links. Matrix (2,5-Dihydroxybenzoic acid) was sublimated to the slides on top of the tissue samples then rehydrated. The matrix assisted laser desorption ionization (MALDI) time of flight (TOF) mass spectroscopy (MS) spectrometer was calibrated and the tissue samples were analyzed.

Discussion

- A novel strategy for imaging intact proteins from human tissue without the need for chemical cross-linking was achieved through the use of the ethanol fixed paraffin embedded tissue samples.
- This work presents a far superior means of visualizing the location of the senile plaques within the human tissue which can benefit future research on targeting the complexity of the amyloid-beta existence.
- While not cross-linked, the ethanol fixed tissue still maintains the benefits of the formalin fixed tissue such as sample lifetime while also improving on the range of analytes that can be investigated.