EU ACADEMY OF SCIENCES

EUAS

EU ACADEMY
2024 ANNUAL REPORT

The President of EUAS

Professor E.G. Ladopoulos

& The Board Governors of EUAS

Contents

"Energy World" by "Universal Mechanics"- The Leading Theory of the Millenium

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 500 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, even approaching the speed of light, the leading technology of ***"Universal Mechanics"*** is proposed and investigated. The groundbreaking theory of *"Universal Mechanics"* consists to 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. Consequently, 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.

When approaching the speed of light an "***Energy World"*** would appear. Is that possible ? Yes of course it is possible. During the past years 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. Hence, if the spacecraft exceeds the speed of light, then it becomes an energy spacecraft. In that case an "***Energy World"*** would be possible.

Another question is what will be next ? Has the energy world to do anything with the life after death ? So, is the soul a kind of energy ? Could be the soul connected to the energy world ? Also, the theory of the "***Energy World"*** in connection with ***"Universal Mechanics"*** is the leading theory of the Millenium.

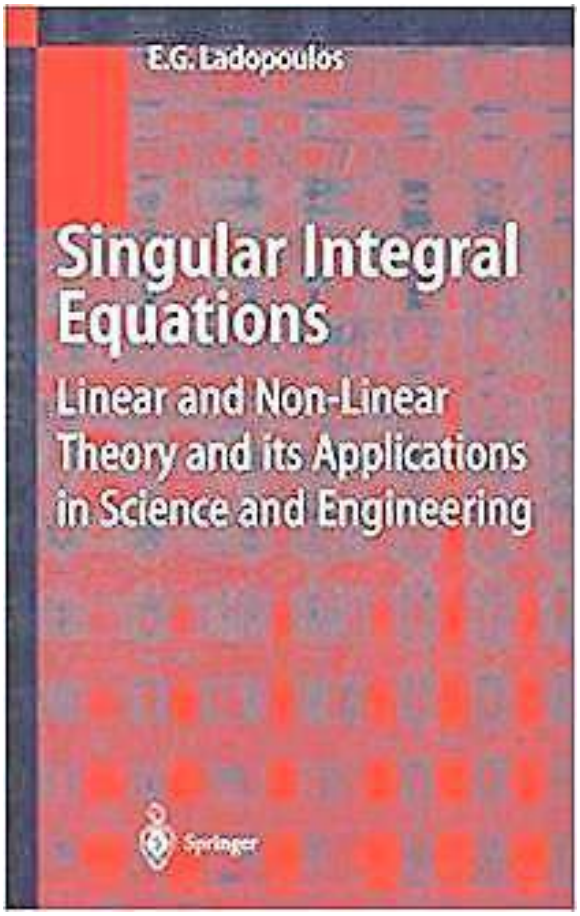
The theory of *"Relativistic Elasticity"* is a combination between the theories of "Classical Elasticity" and "Special Relativity" and results in the ***"Universal Equation of Elasticity"***. Furthermore, the theory of *"Relativistic Thermo-Elasticity"* is a combination between the theories of "Classical 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"***. Hence, 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"***.

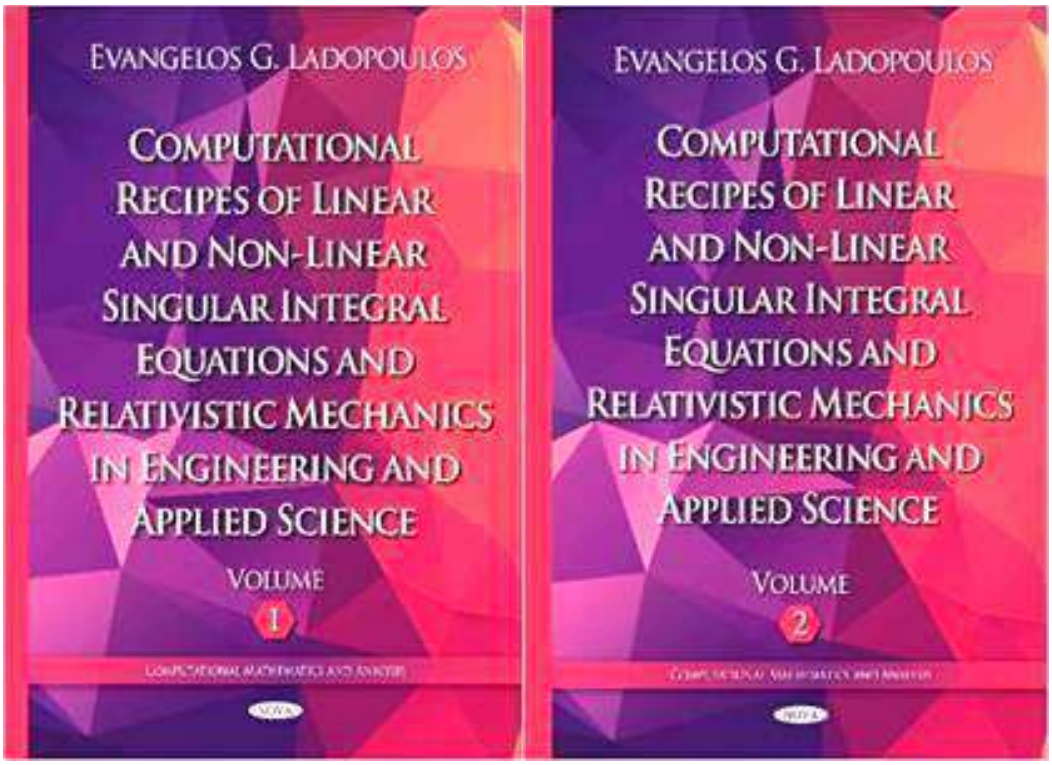
The scope by the International Space Agencies is to achieve in the future, a new generation spacecraft moving with very high speeds, even approaching the speed of light. How far could be this future ? According to current author's research such future could be much closer than everybody believes. For 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. In our published theory there is a lot of ***confidential information***. So, if Space Agencies would be interested for the application of our theory, should come in contact directly with us and not through our publications to try to get some groundbreaking information.

Additionally, 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 with photonics. Laser is light and so their speed is the speed of light. So, the use of laser engines for the future spacecraft might be the best device. The study of such laser engines with photonics is under investigation. Besides, special material should be used for the construction of such spacecraft. Such special meterial is under study and investigation.

A second question is the following: What happens with our leading 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 than light ? 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. Thus, 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.

More details can be seen by the following books:


E.G. Ladopoulos
Singular Integral Equations
Linear and Non-Linear Theory and its Applications in Science and Engineering
Springer


EVANGELOS G. LADOPOULOS
COMPUTATIONAL RECIPES OF LINEAR AND NON-LINEAR SINGULAR INTEGRAL EQUATIONS AND RELATIVISTIC MECHANICS IN ENGINEERING AND APPLIED SCIENCE
VOLUME 1
EVANGELOS G. LADOPOULOS
COMPUTATIONAL RECIPES OF LINEAR AND NON-LINEAR SINGULAR INTEGRAL EQUATIONS AND RELATIVISTIC MECHANICS IN ENGINEERING AND APPLIED SCIENCE
VOLUME 2

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

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

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

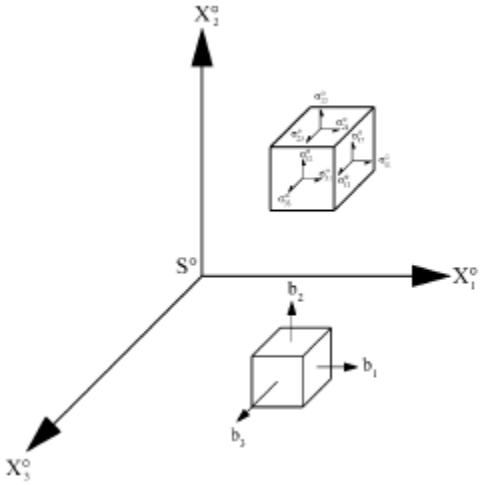


Fig. 1 The state of stress σ_{ik}^0 in the stationary system S^0.

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

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

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

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

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).

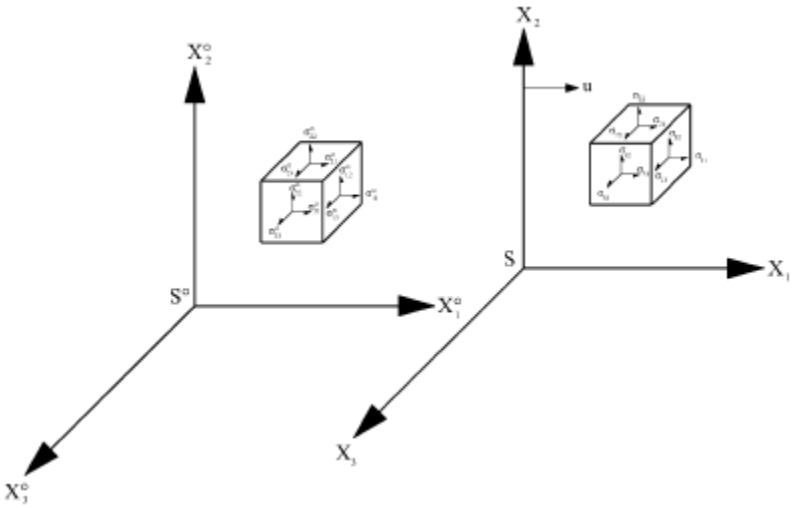


Fig. 2 The state of stress σ_{ik}^{0} in the stationary system S^{0} and σ_{ik} in the airframe system with velocity u parallel to the x_1 - axis.

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***:

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

in which γ is given by:

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

with c the speed of light.

In addition, 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:***

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

where **u** denotes the velocity of the matter at the place and time considered, **σ** the relative stress tensor, $m = E/c^2$ is the total mass density and **ξ** is given by:

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

with **V** the four vector.

Beyond the above, ***"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. Thus, by the current author is completed the theory of Albert Einstein for the whole universe regarding mechanics engineering behavior. ***So, this theory could be the leading Theory of the Millenium.***

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. In addition, 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. So, 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. Consequently, 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. The material which can be used is under investigation.

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

Liquid Crystals: Physics and Applications

by Vladimir Chigrinov, Member EUAS

Short Biography

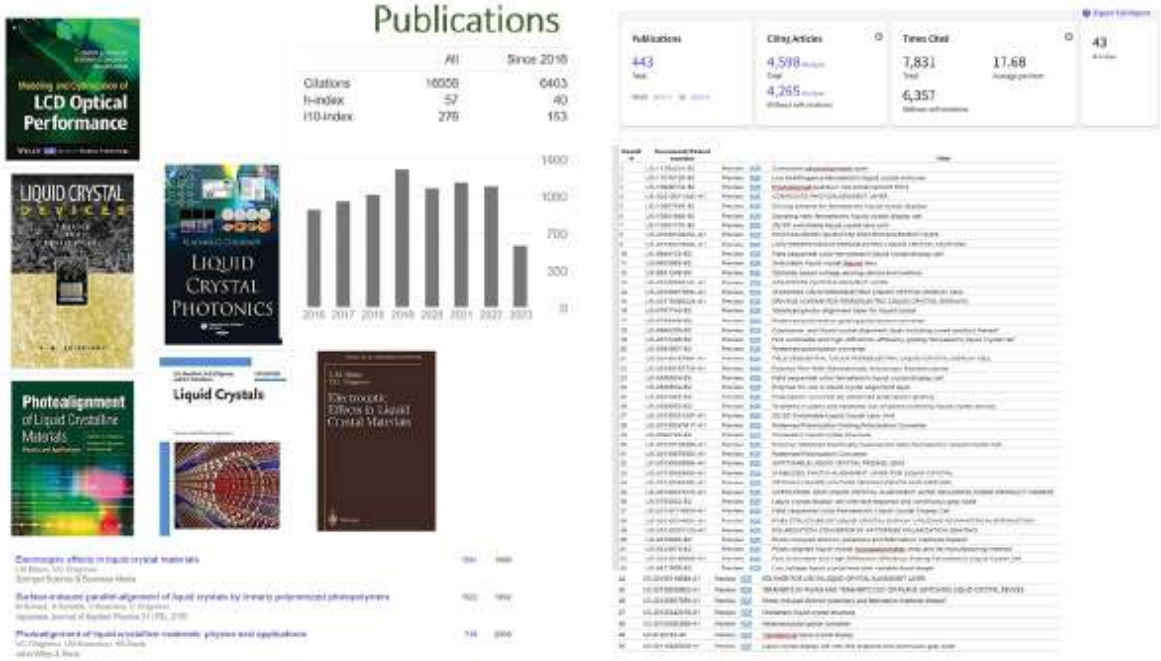
Professor Vladimir G. Chigrinov is Professor of Hong Kong University of Science and Technology since 1999. He is an Expert in Flat Panel Technology in Russia, recognized by the World Technology Evaluation Centre, 1994, and SID Fellow since 2008. He is an author of 6 books, 31 reviews and book chapters, about 334 journal papers, more than 732 Conference presentations, and 121 patents and patent applications including 50 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

Since 2018 he works as Professor in the School of Physics and Optoelectronics Engineering in Foshan University, Foshan, China. 2020-2024 Vice President of Fellow of Institute of Data Science and Artificial Intelligence (IDSAI) Since 2021 distinguished Fellow of Institute of Data Science and Artificial Intelligence.

He is IETI Fellow (https://www.ieti.net/pro/memberdetail.aspx?ID=539) since 2019.

He is a Editor in Chief of Liquid Crystal section in Crystals journal since 2023 https://www.mdpi.com/journal/crystals/sectioneditors/liquid_crystals

Currently he is Emeritus Professor in Hong Kong University of Science and Technology



RESEARCH INTERESTS

- Computer modeling of various electrooptical effects in Liquid Crystals (LC).
- Liquid crystals: physics and applications.
- Photo-aligning and photo-patterning by azodye nanolayers technique for LC application in displays and photonics such as: (i) fast high resolution LC display devices, such as field sequential color ferroelectric LCD; (ii) LC sensors, including LC biosensors; (iii) LC lenses with a variable focal distance; (iv) LC E-paper devices, including electrically and optically rewritable LC E-paper, fast bi and multistable ferroelectric LC devices; (v) photo induced semiconductor quantum rods alignment for new LC display applications; (vi)100% polarizers based on photoalignment; (vii) LC smart windows based on photopatterned diffraction structures; (vii) LC antenna elements with a voltage controllable frequency; (viii) security films.
- LC devices in fiber optics: LC based bandgap fibers, Spectral filters, Tunable waveplates, Tunable gratings, Polarimeter, beam steering devices

The following research has been done recently (year 2024):

Papers

1.Aleksey Kudreyko, Vladimir Chigrinov, Kristiaan Neyts, Denis Chausov and Arina Perestoronina, Photonic Devices with Multi-Domain Liquid Crystal Structures, Crystals, 2024.
2. Efim I. Kats, Vladimir E. Dmitrienko, Eugene M. Terentjev, Vladimir G. Chigrinov, Mikhail A. Osipov, Maxim V. Gorkunov, Anna S. Gorkunova, Boris I. Ostrovskii & Elena S. Pikina, Professor Sergey Alekseevich Pikin (1941 – 2024), Liquid Crystals Today, June 2024.

Conference

1. Vladimir G. Chigrinov, Keynote Talk , Photoaligned Azodye Nanolayers: New Liquid Crystal Alignment Technology, Nano Techforum 2024, Nano Science and Nano Technology, March 2024.
2. Vladimir G. Chigrinov, Liquid Crystal Photoalignment by Azodye Nanolayers: Physics and Applications, Sensor Meet 2024 , Webinar, March 2024.
3. Vladimir G. Chigrinov , Azodye photoaligned nanolayers for liquid crystals Devices, World Nanotechnology Conference, Singapore, March 2024.
4. Vladimir G. Chigrinov, Keynote Talk , Liquid Crystal Azodye Photoalignment: Physics and Applications, Catalysis and Chemical Engineering, Chemical Science 2024, March 2024.
5. Vladimir G. Chigrinov, Keynote Talk , Liquid Crystal Photoalignment by Azodye Nanolayers: New Liquid Crystal Photonics Devices, Optics, Lasers and Photonics Intern. Conf, Barcelona, Spain, March 2024.
6. Vladimir G. Chigrinov, New Liquid Crystal Devices based on Nanosize Photoaligned Azodye Layers, Materials Science Conference, April 2024.
7. Vladimir G. Chigrinov, Invited Talk, Liquid Crystal Photoalignment by Azodye Nanolayers: New Liquid Crystal Photonics Devices, ICDT 2024, Hefei, China, April 2024.
8. Vladimir G. Chigrinov, Liquid Crystals on Azodye Nanolayers: New Trends, Optics Meet 2024 webinar, April 2024.
9. Vladimir G. Chigrinov, Liquid Crystals Photoaligning and Photopatterning on Azodye Nanolayers, Nanotech 2024, Global Cogress on Nanotechnology and Nanomaterials, April 2024.
10. Vladimir G. Chigrinov Keynote Talk ,Azodye photoaligned nanolayers for liquid crystals: physics and applications, Material Science and Nanotechnology, May 2024.
11. Vladimir G. Chigrinov Keynote Talk, Modeling and optimization of liquid crystal display and photonicd devices, 2024 Int. Conf. on Intelligent Optimization and Big Data Management, Wuhan, June 2024.
12. Vladimir G. Chigrinov, Photoaligning and Photopatterning of Liquid Crystals on Azodye Nanolayers: Physics and Applications, International Congress on Optics, Electronics, and Optoelectronics, Wuhan, June 2024.
13. Vladimir G. Chigrinov Keynote Talk, Azodye photoaligned nanolayers: new liquid crystal technology, Smart Masterials 2024, July 20

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Certificate of Recognition

This Certificate is Presented to

Prof/Dr/Mr/Ms. Vladimir G Chigrinov

Hong Kong University of Science and Technology, Hong Kong

in recognition of his/her Plenary Talk on
"Liquid Crystal Photoalignment by Azodye Nanolayers"
at 2nd International Meet on Catalysis, Chemical Engineering and Technology (CATALYSISMEET2024)
Virtually held on July 8, 2024

CERTIFICATE
OF RECOGNITION

Magnus Group Conferences and Organizing Committee
wish to thank

Prof/Dr/Mr/Ms. Vladimir Chigrinov

The Hong Kong University of Science and Technology, Hong Kong

for phenomenal and worthy Oral presentation
at the "8th Edition of World Nanotechnology Conference" held on March 18-20, 2024
in Singapore and Online

Materials Science Conference

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new liquid crystal devices"

Dr. Marta I. Litter

Materials Science Conference-Global Edition
Organizing Committee Members

РОССИЙСКАЯ ФЕДЕРАЦИЯ

ПАТЕНТ

НА ИЗОБРЕТЕНИЕ
№ 2814855

Принтер для пассивной электронной перезаписывающей бумаги на основе азо-красителей с использованием эффекта фотоориентации

Правообладатель: федеральное государственное бюджетное образовательное учреждение высшего образования "Государственный университет просвещения" (RU)

Авторы: Чаусов Денис Николаевич (RU), Курилов Александр Дмитриевич (RU), Белянс Виктор Васильевич (RU), Чигринов Владимир Григорьевич (RU)

Заявка № 2022133524
Приоритет изобретения 13 декабря 2022 г.
Дата государственной регистрации в Государственном реестре изобретений Российской Федерации 05 марта 2024 г.
Срок действия исключительного права на изобретение истекает 13 декабря 2042 г.

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IETI
Technology and Innovation Reward Committee

IETI Industry Innovation Award

IETI Industry Innovation Award Certificate

This certificate is awarded to

Vladimir Chigrinov, Kristiaan Neyts and Aleksey Kudreyko

for outstanding achievement and innovation in the field of Technological Innovation with the project titled ***Computer Simulation and Fiber Optics for LC Devices***. The recipients have demonstrated remarkable ingenuity, dedication, and forward-thinking in bringing about significant advancements and contributions to the industry and IETI, and is hereby recognized with the **Second Prize** of the IETI Industry Innovation Award.

Url: http://www.ietisociety.org/tiarca/202401.html

Date: July 28, 2024

by IETI Technology and Innovation Reward Committee

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President of IETI Council: Prof. Dr. Yong Cao

Research Projects at the Laboratory of Active Controls, Avionics and Aeroservoelasticity Larcase

by Ruxandra Botez, Member EUAS

Short Biography

Dr Ruxandra Botez has finalized her Master's in Engineering in Bucharest, Romania at the Faculty of Aerospace Engineering in 1984, her Master's in Applied Sciences in Ecole Polytechnique in Montreal, Canada in 1989 and her PhD in McGill University in Montreal, Canada in 1994. She worked at the ICA-Brasov Factory of Helicopters on the Puma and Alouette helicopters development in Romania (1984-1987) and at Bombardier Aerospace in Aircraft Engineering in Montreal as AeroServoElasticity task leader during 1995-1997. She worked as a Postdoctoral Fellow at Auburn University during 1994-1995, and she is a Full Professor at École de technologie supérieure (ÉTS), part of the Quebec University in Montreal, Canada since 1998.
Ruxandra is the Editor-in-Chief of the INCAS Bulletin and Associate Editor of 10 other journals including the Aeronautical Journal. Ruxandra graduated more than 460 students in her academic career, who worked on her research projects: 27 PhD students, 140 Master's students (projects and theses) and 300 Internship students. Ruxandra published more than 200 archival original journal articles, 320 conference papers and 7 invited book chapters.
Ruxandra and her team have obtained more than 70 awards; she also gave more than 50 invited speaker presentations. Ruxandra's projects were and are realized in collaboration with aerospace companies well-known internationally, such as Bombardier, CAE, CMC Electronics, Bell Helicopter Textron, Thales Aerospace, GlobVision, FLIR Systems, Presagis, Alenia, Hydra Technologies, as well as with research institutes, such as IAR-NRC, and NASA, and CIRA, DLR, INCAS, and with various Canadian and international universities.
Ruxandra is a Fellow of the American Institute of Aeronautics and Astronautics (AIAA), the Canadian Academy of Engineering (CAE), Canadian Aeronautical Society Institute (CASI), Royal Aeronautical Society (RAeS), International Association of Advanced Materials (IAAM), International Artificial Intelligence Industry Alliance (AIIA) and Asia-Pacific Artificial Intelligence Association (AAIA).
Ruxandra is a Full Member of the American Romanian Academy of Arts and Sciences (ARA), and Member of the American Society of Mechanical Engineers (ASME), Vertical Flight Society (VFS) International, Society of Automotive Engineering (SAE) International, and Romanian Academic Association of Canada (RAAC).
Ruxandra is an Honorary Foreign Member of the Romanian Academy, and an Honorary Member of the International Sustainable Aviation and Energy Research Society.
Ruxandra is the Canada Research Chair Tier 1 Holder in Aircraft Modeling and Simulation Technologies since 2011, and she is the Founder and Head of the Laboratory of Applied Research in Active Controls, Avionics and AeroServoElasticity LARCASE since 2003, where more than 45 students and researchers work every semester on various projects.

In Section 1 of this article, the LARCASE infrastructure and equipments are described, and their photos are presented in Appendix 1. In Section 2, some of the research projects realized using these equipments are presented.

1. The LARCASE Equipements

There are four main equipments at the LARCASE that are used mainly in the Canada

Research Chair in Aircraft Modeling and Simulation New Technologies. Three of these large-scale equipments were obtained with research grants from the Canadian Foundation of Innovation CFI, the Ministère du Développement Économique, Innovation et Exportation MDEIE; all of them were specially designed and manufactured for LARCASE research needs, while the fourth equipment was a donation. These equipments are explained in the next paragraphs of this section.

In 2009, the first important infrastructure equipment was obtained from CAE and Cessna, called the Research Aircraft Flight Simulator (RAFS). This equipment has an open-source code for the flight dynamics of the Cessna Citation X (CCX) business aircraft, which is one of the fastest aircraft in its category; the flight dynamics has the highest-Level D Federal Aviation Administration (FAA) certification, and for this reason, this simulator is extremely helpful in the advancement of aircraft modelling and simulation.

Professors Michael Païdoussis and Stuart Price have donated in 2010 the large blow-down subsonic wind tunnel, developed and used at McGill University by them to be used at the LARCASE.

The Research Aerial System (RAS) was obtained in 2011 at LARCASE. The RAS is based on the Unmanned Aerial System UAS-S4 Éhecatl, and it was designed, developed and manufactured by the Mexican company Hydra Technologies. The UAS-S4 is used extensively by the Police and the Air Forces in Mexico, which justifies its high scientific quality, reputation and reliability.

In 2019, Dr. Botez has successfully obtained an important infrastructure equipment from CAE and Bombardier, called the Virtual Research Simulator (VRESIM). This equipment has an open-source code for the flight dynamics of the CRJ-700 regional transport aircraft; the flight dynamics has the highest-Level D FAA certification, and for this reason, this simulator is extremely helpful in the advancement of Bombardier type aircraft modelling and simulation.

The Appendix 1 shows all these equipments, that are also found on the LARCASE website in the Equipments section.

These equipments are unique in the academic environment, mainly because of the flight test data confidentiality in companies and therefore, these equipments are difficult to obtain in universities. The RAFS, VRESIM and RAS are unique as they were developed by industrial partners (CAE, Bombardier, Cessna and Hydra Technologies) for the LARCASE team research needs. From our knowledge, the LARCASE is the only aerospace academic laboratory to presently have this type of research equipements combination.

2. Research Contributions and Projects at the Larcase

Various research contributions were done at the LARCASE in the areas of aircraft design, modeling and simulation at both theoretical and practical levels in areas, such as: (i) advanced flight dynamics and control methodologies, (ii) active control technology and morphing applications for aircraft using aeroservoelasticity knowledge, iii) flight trajectories optimization for Flight Management Systems (FMS), and other related areas.

These methodologies have been experimentally validated using both flight and wind tunnel tests. These types of research have been performed on flying vehicles, such as rotorcraft, aircraft, and unmanned aerial vehicles with the global aim of advancing Green Aircraft Technology.

These projects were done in collaboration with teams working in different world-renowned aerospace companies, such as Bombardier Aviation, Bell Textron, Canadian

Aviation Electronics (CAE), CMC Electronics (in Canada), Thales Group (in Canada and France), Presagis (in the USA), Leonardo Aerospace (in Italy), Hydra Technologies (in Mexico), research institutes, such as the Institute for Aerospace Research - National Research Council IAR-NRC (in Canada), Italian Aerospace Research Centre CIRA (in Italy), National Institute for Aerospace Research "Elie Carafoli" INCAS (in Romania), National Aeronautics and Space Administration NASA (in the USA), and with academic partners from ÉTS, Polytechnique Montreal, McGill, Concordia and Carleton universities (in Canada), in Europe with the University of Craiova and Academia Militara Tehnica "Ferdinand I" (in Romania), École d'ingénieurs ÉPF (previously: École polytechnique féminine) and Isae-ESTACA (École supérieure des techniques aéronautiques et de construction automobile) in France, University of Bologna and University of Naples Federico II (in Italy), and from Sao Paulo State University UNESP (in Brazil). Ruxandra and her team have also worked on several projects funded by the North Atlantic Treaty Organization NATO that took place in collaboration with partners from many countries. In this section, we present work performed mainly using the research equiments existing at the LARCASE.

2.1 Example of research performed on the RAFS of the Cessna Citation X

The RAFS for the CCX has been used at the LARCASE with the aim of designing a highly efficient aero-propulsive model from a minimum available flight test data for the climb, cruise and descent (including acceleration and deceleration) regimes. The maximum modeling error was found to be, according to the FAA criteria, smaller than 5%. The novelty of the research consisted in the fact that the aerodynamic coefficients or engine data were not used. Excellent results (fitting between the model and flight test data of 98%-100%) were obtained using the RAFS for the CCX.

This aero-propulsive model could be generalized for all flight conditions, and further improved for other types of business aircraft. The main motivation of this type of research was the development of an aero-propulsive efficient model (for overall greenhouse and fuel emissions reduction) based on a minimum available amount of data, such as the ones provided by the Aircraft Flight Manual (or equivalent).

This type of research, oriented towards highly efficient aero-propulsive aircraft modeling, is extremely useful for aircraft manufacturers, such as Bombardier, Boeing, Airbus, Cessna, as it conducts to the reduction of the number of flight tests (and thus, the costs) required for their prototype validation. This research is also extremely helpful to sub-contractors in avionics systems (FMS, GPS, etc), such as CMC Electronics, and to aircraft modeling and simulation companies, such as CAE Inc. and Thales, as the models developed at the LARCASE are based on a minimum available data required from aircraft manufacturers; it is known that these companies need to acquire flight test data to complete their database information in order to improve their in-house aircraft or avionics systems models, which is very expensive for them. As the aero-propulsive models developed by LARCASE need a minimum amount of data, then, these companies could develop their models faster and better based on a minimum of information and flight tests, which could conduct to fewer flight tests, that would result in fuel consumption reduction, therefore, in important economic benefits.

Performance monitoring and automatic model updating of the CCX aircraft have also been performed. New algorithms were developed for predicting the performance and flight trajectories of the CCX aircraft, which considered wind effects and piloting techniques in

various flight phases. New modern robust control methodologies for the CCX aircraft were also developed and validated using also artificial intelligence techniques.

The "Morphing Winglet" and "Morphing Horizontal Tail" concepts were studied and analyzed to improve the aerodynamic performance of the CCX aircraft. The horizontal stabilizer ("Morphing Horizontal Tail") of the CCX aircraft was able, through the use of a new optimization methodology, to change its shape and balance the aircraft itself in order to reduce drag and therefore fuel consumption during cruise flight. An average fuel consumption reduction of 4% was achieved for the cruise flight cases. The methodologies and results of this research using the RAFS was published in Refs. 1-19, as well as in many conference proceedings papers.

2.2 Example of research performed on the VRESIM of the CRJ-700

New methodologies for the CRJ-700 regional commercial aircraft and its engine were developed in the areas of aero-propulsive modeling and simulation based on flight tests and geometric data. New control methodologies were developed and validated using the VRESIM simulator. The "Morphing Winglet" aspects of this regional aircraft were studied and analysed.

Modelling the aerodynamic characteristics of an aircraft under stall conditions remains a very important study for engineers and researchers. A new methodology for modeling aerodynamic coefficients and predicting flight dynamics of the CRJ-700 aircraft under static and dynamic stall conditions, including linear and nonlinear phases (as well as the hysteresis cycle) has been developed based on neural networks. The collected data was then used to create a database of aerodynamic coefficients for the entire flight envelope of the aircraft. The models were then integrated into a Matlab/Simulink simulated CRJ-700 aircraft platform to validate their design. The flight parameters predicted by the platform were compared with those obtained by the VRESIM simulator. The criteria used to validate the model were defined by the FAA, which specified the tolerances required for estimating the angles of attack, pitch angles, true airspeeds, and altitudes for both dynamic and static stall phases. All validation flight tests gave excellent results with a 100% success rate, i.e. the simulation platform results were identical to those collected by the VRESIM.

The CRJ-700 aircraft engine performance model was identified from flight test data for a wide range of operating conditions using *Neural Network* methods. The data collected for the take-off, climb, cruise and descent phases were then used to create a database for the training process. The validation of the methodology was performed by comparing the prediction model with a set of flight data collected using the VRESIM. The results showed that the model was able to predict the engine performance as a function of RPM, thrust and fuel flow with excellent accuracy.

In addition, the optimization aspects of the "Morphing Winglet" of this regional aircraft were studied and analyzed. This wing model for the CRJ-700 demonstrated its strength at maximum aerodynamic loads, as well as at load factors between -2G and 7G, while the maximum lift to drag ratio was increased by 4%. The methodologies and results of this research using the VRESIM was published in Refs. 20-30, as well as in many conference proceedings papers.

2.3 Example of research performed using the Unmanned Aerial Systems UAS-S4 and UAS-S45

Research on UAS-S4 and UAS-S45 morphing wing systems involves MultiDisciplinary

Optimization (MDO) knowledge in the areas of aerodynamics, structure and control. Original methodologies have been developed for the aerodynamic and structural analysis of unconventional designs of both UAS-S4 and UAS-S45. Therefore, a new nonlinear Vortex Lattice method in aerodynamics has been developed at the LARCASE to optimize the UAS-S4 wing model at large angles of attack, close to dynamic loss-of-balance conditions.

In parallel, structural studies, including moment of inertia computations for the S4 and S45 UASs, were performed and the modelling of these systems was mainly based on semi-empirical methodologies. Various other aerodynamic optimisation methodologies were developed to improve their aerodynamic performance. For various new concepts of optimised and morphing configurations of these systems and different flight conditions, the following maximum performances were obtained by comparing them with the initial ones: drag reduction by 4.5%, delay of boundary layer separation by 15% of the wing airfoil chord, stall angle delay by 3^0, increase of lift to drag ratio, expressed by $CL^{3/2}/CD$ ratio, by 10.25%, and increase of lift by 26% and maximum lift by 9.6%. It was concluded that morphing UAS technologies are highly beneficial.

A flight dynamics simulator was also designed and developed by Dr. Botez' team for both UAS-S4 and UAS-S45. This modelling is extremely useful for the Mexican company Hydra Technologies as it could be used for pilot training and for improvement of their modeling, simulation and control methodologies. The flight simulator technology research methodologies and results could also be used by other UAV designers and manufacturers. The methodologies and results of this research using the RAS for the UAS-S4 and UAS-S45 was published in Refs. 31-61, as well as in many conference proceedings papers.

2.4 Example of research performed using the Price-Païdoussis Subsonic Wind Tunnel

The Price-Païdoussis Subsonic Wind Tunnel is used for analyzing and testing of aerodynamics, structure and controls concepts of reduced scale morphing wings and their components on the ATR-42 aircraft, UAS-S4 and UAS-S45. The Morphing Leading Edge (MLE), Morphing Trailing Edge (MTE) and Morphing Camber System (MCS) concepts were studied, analyzed and experimentally tested.

New calibration technologies using artificial intelligence, such as *Neural Network* and *Extended Great Deluge* were also performed. Aerodynamic studies were also done on two FLIR Systems Radars R20SS and R6 to test their aerodynamic resistance to the winds, and they were successfully experimentally tested in the Price-Païdoussis subsonic blow down wind tunnel at the LARCASE. For this project, a third test section was designed and fabricated for use in the LARCASE wind tunnel. The numerical aerodynamics results were validated with experimental wind tunnel tests data.

Nonlinear adaptive fuzzy control methodologies were used to analyze the chaotic uncertainties of flapping wings. The wind tunnel was used also to validate experimentally the flapping wings dynamics in collaboration with Professor Païdoussis from McGill.

Another interesting research tested in the wind tunnel was performed in collaboration with professor Rachid Aissaoui from the LIO (*Laboratoire de recherche en imagérie et orthopédie*) at ÉTS in the biomedical field by studying the effects of the winds on the human walking. The methodologies and results of this research using the subsonic wind tunnel were published in Refs. 62-72, as well as in many conference proceedings papers, while Ref. 73 gives also other details of the LARCASE research work.

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Appendix 1
LARCASE Infrastructure

Figure 1. Research Aircraft Flight Simulator (RAFS) for the Cessna Citation X Business Aircraft (developed in collaboration with CAE and Cessna)

Figure 2. Virtual Research Flight Simulator (VRESIM) for the CRJ-700 Aircraft (developed in collaboration with CAE and Bombardier)

Figure 3. The autonomous aerial unmanned system UAS-S4 developed by Hydra Technologies

Figure 4. Price – Païdoussis Subsonic Blowdown Wind Tunnel (McGill University donation from Professors Michael Païdoussis and Stuart Price)

Next Investigations 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 two times six weeks working at Philips Natuurkundig Laboratorium, Eindhoven, The Netherlands. As a research associate, he was at M.I.T 1964-1965 where he earned a M.Sc. degree in microwaves, and at Stanford University 1965-1966, both years in radioastronomy. Back in Belgium in 1966, he founded the Microwave Laboratory at UCL, which he headed for 35 years. His research interests concentrated successively on 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 satellite communications. He supervised 27 doctoral theses and about 200 engineer's theses.

Prof. Vander Vorst has authored and co-authored eight books, a number book chapters, and more than 400 papers in peer-reviewed journals and conference proceedings. His penultimate book, RF/Microwave Interaction with Biological Tissues with A. Rosen and Y. Kotsuka as co-authors, was published in 2006 by Wiley, U.S.A. He recently co-authored papers on various websites on the 5G, the effect of electromagnetics on viral infections, and electro-hypersensitivity and how to cure it. He has written chapters on bioelectromagnetics in a collective book investigating electro-hypersensitivity and papers on the same subject.

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 60 years, Prof. Vander Vorst has been actively involved in developing the international microwave community. In 1967-2001 he chaired 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. He 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 and is still active with EuMA.

Prof. Vander Vorst also served the 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. He obtained a number of awards including the Microwave Career Award 2004 from I.E.E.E MTT-S, the Distinguished Service Award 2016 from EuMA and the Propagation Award 2019 from the European Association for Antennas and Propagation (EurAAP).

He is an emeritus member of Belgian Academia of Letters and Science, a member of Academia Europaea, the Electromagnetics Academy, and the EU Academy of Sciences. He is a Honorary Member of the Belgian National Committee or URSI and of a number of international committees. 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, twelve grandchildren and five great-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 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 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 several PhD students in their doctoral thesis and later.

Site-shielding, specifically 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 a doctoral thesis on three experimental steps.

The first research 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].

Fig. 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 implanted 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 another doctoral thesis. 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 a doctoral thesis. 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 *RF/Microwave interaction with biological tissues* was written and published by Wiley U.S. in 2006, with A. Vander Vorst, A Rosen and Y. Kotsuka as co-authors, and with PhD students as a prime target [36]. During the last five years, A. Vander Vorst co-authored papers on various websites on 5G, on the effect of electromagnetics on viral infections, and on electro-hypersensitivity. He wrote chapters on bioelectromagnetics (em) and bioelectromagnetic interaction with the human body in a collective book investigating **electro-hypersensitivity** (EHS) [37]. He is a co-author of a review paper on the importance of molecular biomarkers and imaging in the study of EHS [38]. Over the last years, he co-authored about twenty letters concerning em in hospitals on one hand [39] and em interaction with the human body on the other [40].

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Ultra-effective Room Temperature Gas discrimination based on Monolithic Pd@MOF-derived Porous Nanocomposites: an exclusive scheme with Photoexcitation

by Jinhua Sun, Member EUAS

Short Biography

Education and Positions

2022~ Chair Professor, University of Science and Technology of China
2019~ Chairman, Sub-Academic Advisory Committee of USTC
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

Fellow Selection Committee Member, The Combustion Institute (2024~)
Executive Officer Nomination Committee, The Combustion Institute (2023)
Vice-chairman of Electrical Fire Protection Committee, CFPA (2021~)
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 (2008~2022)
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 six International Journals (2010~)

Editorial Board of nine national Journals (2003~)
Academic Committee Member of China Fire Protection Association (2003~2020)
Honors and Awards
Serving-the-people Award, USTC (2024)
Science and Technology Award, First-class Award, Anhui Province (2024)
Fellow of The Combustion Institute (2023)
Model Research Worker Award, Anhui Province, China (2022)
Science and Technology Award, Second-class Award, Anhui Province (2022)
Moral Model of Teacher Award, Anhui Province, China (2021)
Lifetime Contribution Award of AOAFST (2021)
Science and Technology Progress Award, First-class Award, CAPS (2021)
Special government allowance of the State Council, The State Council of the P. R. China (2019)
Science and Technology Innovation Award, First-class Award, CFPA (2018)
Science and Technology Progress Award, First-class Award, China Highway and Transportation Society (2018)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2017)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2017)
Zhu Li Yuehua excellent teacher Award, Chinese Academy of Sciences (2014)
Excellent graduate student supervisor Award, Chinese Academy of Sciences (2014)
Teaching Award of Anhui Province, First-class Award, Anhui Province (2010)
Beijing Science and Technology Award, Third-class Award, Beijing (2008)
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)
National Science and Technology Progress Award, Second-class Award, China (2006)
Outstanding Member of Hundred Talent Program, Chinese Academy of Sciences (2005)
Member of Hundred Talent Program, Chinese Academy of Sciences (2001)
National Science and Technology Progress Award, First-class Award, China (1993)

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, general projects of NSFC, and "Outstanding Talents" project funded by the Chinese Academy of Sciences.

Prof. Sun has published more than 450 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 20,000 times (Web of Science). Contributions have also been recorded in 11 academic books or book chapters and over 60 keynote or invited talks at national or international conferences. In addition, Prof. Sun has supervised over 60 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 2024

1. **Peiyu Duan, Haowen Wang, Qingkui Peng, Shiyao Chen, Hongmin Zhou, Qiangling Duan, Kaiqiang Jin and Jinhua Sun*., Ultra-effective room temperature gas discrimination based on monolithic Pd@MOF-derived porous nanocomposites: an exclusive scheme with photoexcitation. *Journal of Materials Chemistry A*, 2024, Volume 12, 3896-3909.**

   Chemiresistive sensing materials capable of efficiently identifying specific flammable gases are imperative. Althoughplenty of high-performance chemiresistive sensorshave been developed in related fields, the high selectivity response to a single flammable gas at room temperature is still a great challenge. Conventional single chemiresistive metal oxide semiconductor materials exhibit similar response characteristics to flammable gases at high temperatures, while arrays are limited by high cost and miniaturization. Herein, the unique gas discrimination based on a monolithic MOF-derived chemiresistive sensor is achieved with photoexcitation at room temperature. 5.0Pd@ZnO exhibits a typical p-type semiconductor response (200 ppm, 52.89) to H 2 , while it displays a typical n-type semiconductor response to other flammable gases (CO, MeOH, EtOH, and H 2 S response of −25.15, −13.63, −49.92, and −40.36, respectively), which indicates that H 2 can be fully identified merely from the original electrical signal. Meanwhile, the as-prepared sensors combined the advantages of MOF and MOS materials, and exhibited high linearity response, favorable repeatability, and long-term stability. The special response characteristics of the sensor to each flammable gas have been explored in detail, and the distinct effects of two different Pd surface states on gas molecules are discovered by DFT calculations. The mechanism of the high-selectivity response behavior at room temperature is systematically analyzed. This work provides a solid reference and feasible solution for the development of high-selectivity room temperature sensors.

2. **Junyuan Li, Peng Gao, Bang Tong, Zhixiang Cheng, Mingwei Cao, Wenxin Mei, Qingsong Wang, Jinhua Sun a** , Peng Qin*, Revealing the mechanism of pack ceiling failure induced by thermal runaway in NCM batteries: A coupled multiphase fluid-structure interaction model for electric vehicles, *eTransportation* 20 (2024) 100335.**

   Structure failure of lithium-ion battery (LIB) pack ceiling leads to the unintended release of combustible and poisonous substances during thermal runaway (TR), resulting in personnel injuries and financial losses. However, limited research has been conducted on the mechanism behind pack ceiling failures. In this study, we developed a coupled multiphase fluid-structure interaction (FSI) model to simulate the evolution of up-cover baffle under the TR impact of a 52 Ah NCM battery. Our findings reveal several important insights:1) the maximum force and temperature on the baffle are 13.01 N and 598.5 ◦ C in experiment; 2) the simulation shows that particles exert higher temperature and greater force on the baffle compared to the gas phase; 3) the overall equivalent stress in the stainless-steel baffle surpasses the tensile strength that

incurs crack on the baffles. According to the validated model, we find that the baffle structure failure is caused by the thermal stress from particle-structure heat conduction. Furthermore, this observation is applicable to the structure failure problems associated to the thermal runaway of high-density battery that involves enormous particles. In addition, the insulation layer is found to be more effective than the gap distance in protecting the pack ceiling. These findings offer a valuable insight into the structure design of LIB pack, and provide the guidance toward future battery integration technologies.

3. **Songlin Zhang, Qian Zeng, Jing Tang, Guangbo Jiang, Yiming Jiang, Qiangling Duan*, Jinhua Sun**, Critical criterion for spontaneous ignition of high-pressure hydrogen released into the atmosphere through a tube, *International Journal of Hydrogen Energy* 92 (2024) 342–348.**

Spontaneous ignition induced by high-pressure hydrogen leakage has primarily been discussed qualitatively, focusing on factors such as release pressure, downstream tube size, and the rupture of the burst disk. However, quantitative investigations and prediction models remain limited and unclear. In this paper, we introduce the relative molecular mass M and delve into its influence on the critical pressure threshold for spontaneous ignition of high-pressure hydrogen leaks. Additionally, we introduce the mass flow rate Q, as a metric to quantify the impact of opening area and shape on the ignition process. By integrating six key factors, including tube diameter D, tube length L, atmospheric pressure P a , burst disk opening time t, gas mass flow rate Q, and gas relative molecular mass M, four dimensionless factors affecting the critical leakage pressure were determined by using similarity analysis. The correlation between the dimensionless numbers was verified by correlation analysis and calibrated to the experiments of this paper and other authors. Finally, a critical criterion for spontaneous ignition from leakage in high-pressure hydrogen tubes was established to provide a basis for safety evaluation and prevention techniques for high-pressure hydrogen.

Modeling of Turbulence and in the Modeling of Electrocardiac Physiology

by James Glimm, Member EUAS

Short Biography

Professional Preparation

Columbia University, Engineering, BA, 1956
Columbia University, Mathematics, Ph.D. 1956-1959

Appointments

1999-	*Staff Member, Computational Science Center, Brookhaven National Laboratory*
1989-	*Distinguished Professor, SUNY at Stony Brook*
1982-89	*Professor, Courant Institute, New York University*
1974-82	*Professor, The Rockefeller University*
1968-74	*Professor, Courant Institute, New York University*
1960-68	*Professor, Associate Professor, Assistant Professor, MIT*
1959-60	*Temporary Member, Institute for Advanced Study*

Professional Service

Advisory Committee of the Center for Computational Geoscience, Xi'an University, Xi'an PRC
2007-2009 President American Mathematical Society

Prizes, Awards, Fellowships

2002	*National Medal of Science*
	Member, National Academy of Sciences
	Member, American Society of Arts and Sciences
1993	*Steele Prize for a paper of fundamental importance (AMS)*
1980	*Dannie Heineman Prize for Mathematical Physics (APS)*
1965-1966	*Guggenheim Fellowship*
1963-1964	*Guggenheim Fellowship*
1959-1960	*National Science Foundation Fellowship*

Fields of Expertise

Nonlinear partial differential equations, Computational fluid dynamics, Stochastic partial differential equations, Mathematical physics, Quantum physics, Scientific computing, Quantification of uncertainty, Turbulence modeling, Computational electromagnetics, Turbulence modeling, Financial mathematics

My contributions have been highly cited and honored across a wide spectrum of scientific disciplines, starting with mathematical analysis, followed by nonlinear partial differential equations. My leading contributions to the mathematical formulation of quantum field theory and statistical physics are widely noted. I have made fundamental contributions to uncertainty quantification, in application to flow in subsurface acquifers and petroleum reservoir subsurface flow. I have established expertise in the modeling of turbulent flow with recent work on ventricular fibrillation.

I have two major research areas, in the modeling of turbulence and in

the modeling of electrocardiac physiology (also a form of turbulence, in this case of electrical signals.

We have studied turbulence from multiple points of view, including mathematical theory, analysis of experimental data, and analysis of numerical turbulent simulation data.

The famous Kolmogorov 1941 scaling law $<v(k)^2> \sim C_K \epsilon k^{`5/3}$ led to two mathematical theorems. We assumed such a scaling law, which amounts to the statement that the velocity field lies in a fractional Sobolev space of positive index.

Taking this as an assumption, we derived as a consequence that weak solutions of the Navier-Stokes equation converge strongly in a fractional Sobolev space (via compactness and selection of a convergent subsequence) to a solution of the Euler equations [1]. This result for the incompressible Euler equation was later extended to a similar result for the compressible Navier-Stokes and Euler equations [2].

We have also examined in detail turbulent missing experimental data. We considered a definitive experimental study of Rayleigh-Taylor (RT) acceleration driven turbulent mixing data. Here we disproved a popular but unsupported conjectures that a definitive body of such experiments was heavily influence by noise in the initial interface position, [8]. [4] We developed theoretical analysis method for the analysis of the RT instability. A bubble merger model [5] correctly predicts the α_b parameter and additionally predicts its ratio to the bubble widths. Asymptotic scaling relations are predicted [6], in agreement with experimental parameters. This line of study continues [7] with further and new experimental data.

Our numerical simulations of the RT instabilities have been highly successful. They are based on the dynamic Sub Grid Scale (SGS) methodology developed in the 1990-‘s with a front tracking methodology of our own development [9].
In this combination, we achieved verification and validation of our algorithm, with a recent summary found in [4].

We have been studying electrocardiac physiology, with a focus on the

fibrillation state and the defibrillation protocols used to treat it. My contributions to a number of technologies support these studies. These include uncertainty quantification, numerical algorithm development, high performance simulations and turbulence modeling

A recent paper [9], closely related to the work proposed here, develops methods to generate high resolution cardiac geometry with blood vessels of minimum diameter 50 microns resolved. The construction is based on data from a rabbit ventricle. The main thrust of the paper is methods nearly fully automated, and sufficiently automated to allow extensions to the human heart. We include outer as well as inner blood vessels walls and fibers wrapped around the blood vessels. Portions of these methods were developed in an earlier paper [10]. We also mention the paper [13],

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Seawater Carbonate Chemistry and Diatom Aggregation when exposed to Crude Oil and Chemical Dispersant

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 at Columbia University, N.Y., after graduating from the University of Bern, Switzerland, with a Ph.D. in Chemistry. Dr 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 of well over 300 journal articles and 45 book chapters on these subjects, which, over the years, have received more than 15,000 citations. More on his research can be found at https://www.tamug.edu/mars/faculty-bios/PeterHSantschi.html and https://scholar.google.com/citations?user=ZKGyOTsAAAAJ&hl=en&oi=ao.

*His total of 400+ peer-reviewed publications, according to the ISI Web of Science (all databases as of August 3, 2020), attest to his productivity, while his citation record is a testimony of his impact. Santschi's record is thus not only of quantity alone but predominantly of quality. Metrics establishing scientific impact are difficult to come by, but if the citation count and other indexes (e.g., h-index from ISI, all databases) may serve as a measure of scientific impact, then his 400+ publications have been cited over 17,000 times, with an average citation per publication of over 42. Other indexes for his publications (ISI h-index = 71 and productivity m-index = h/Δt = 1.**51** with Δt = 47 years since the 1st publication in 1974; g-index = 137; and Google Scholar h-index = 87 and i-10 index = 293, with well over 25,000 citations) are exceptional.*

*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 many collaborative and/or supportive scientists.*

***His international pre-eminence** is not only demonstrated by the prestigious awards that he received, but also by the fact that he was invited as a member of 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.** 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, Peter's main contributions and impacts in environmental geochemistry are on the role of macromolecular natural organic matter, 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 tested, before state-of-the-art instrumentation can be applied.*

Abstracts of Recent Publications 2024

1. Genzer, Jennifer L; Kamalanathan, Manoj; Bretherton, Laura; Hillhouse, Jessica; Xu, Chen; Santschi, Peter H; Quigg, Antonietta (2024): Seawater carbonate chemistry and diatom aggregation when exposed to crude oil and chemical dispersant. PANGAEA.

Abstract: Roller table experiments with Thalassiosira pseudonana, a small centric diatom, were conducted to produce marine snow aggregates in six treatments: Control (pCO2 = 400 ppm), OA (pCO2 = 750 ppm), water accommodated fraction of oil (WAF), OAWAF, diluted chemically enhanced WAF (DCEWAF), and OADCEWAF. Measurements included intracellular photophysiological responses, oil concentrations and polycyclic aromatic hydrocarbons (PAHs), aggregate morphology, transparent exopolymeric particles (TEP), and extracellular polymeric substances (EPS) to investigate if OA will affect the response to oil spill conditions. The experiments were conducted in the dark to eliminate cell replication and photosynthesis and used both stationary and exponential growth phases.

2. **Kaplan, D.I., Boyanov, M.I., Losey, N., Lin, P., Xu, C., O'Loughlin, E.J., Santschi, P.H., Xing, W., Kuhne, W., Kemner, K.M. 2024. Uranium biogeochemistry in the rhizosphere of a riparian wetland. ES&T.**

Abstract: The objective of this study was to determine if U sediment concentrations in a U-contaminated wetland located within the Savannah River Site, South Carolina, were greater in the rhizosphere than in the non-rhizosphere. U concentrations were as much as 1100% greater in the rhizosphere than in the non-rhizosphere fractions; however and importantly, not all paired samples followed this trend. Iron (but not C, N, or S) concentrations were significantly enriched in the rhizosphere. XAS analyses showed that in both sediment fractions, U existed as UO_2^{2+} coordinated with iron(III)-oxides and organic matter. A key difference between the two sediment fractions was that a larger proportion of U was adsorbed to Fe(III)-oxides, not organic matter, in the rhizosphere, where significantly greater total Fe concentrations and greater proportions of ferrihydrite and goethite existed. Based on 16S rRNA analyses, most bacterial sequences in both paired samples were heterotrophs, and population differences were consistent with the generally more oxidizing conditions in the rhizosphere. Finally, U was very strongly bound to the whole (unfractionated) sediments, with an average desorption K_d value ($U_{sediment}/U_{aqueous}$) of 3972 ± 1370 (mg-U/kg)/(mg-U/L). Together, these results indicate that the rhizosphere can greatly enrich U especially in wetland areas, where roots promote the formation of reactive Fe(III)-oxides.

3. **Hung, C.-C,, Hsieh, H.-H., Chou, W.-C., Liu, E.-C., Chow, C.H., Chang, Y., Lee, T.-M., Santschi, P.H., Ranatunga, R. R. M. K. P., Bacosa, H.P., Shih, Y.-Y. 2024 Assessing CO_2 sources and sinks in and around Taiwan: implication for achieving regional carbon neutrality by 2050. Marine Pollution Bulletin 206 (2024) 116664.**

Abstract: Taiwan has pledged to achieve net-zero carbon emissions by 2050, but the current extent of carbon sinks in Taiwan remains unclear. Therefore, this study aims to first review the existing nature-based carbon sinks on land and in the oceans around Taiwan. Subsequently, we suggest potential strategies to reduce CO2 emissions and propose carbon dioxide removal methods (CDRs). The natural carbon sinks by forests, sediments, and oceans in and around Taiwan are approximately 21.5, 42.1, and 96.8 Mt-CO2 y 1, respectively, which is significantly less than Taiwan's CO2 emissions (280 Mt-CO2 y 1). Taiwan must consider decarbonization strategies like using electric vehicles, renewable energy, and hydrogen energy by formulating

enabling policies. Besides more precisely assessing both terrestrial and marine carbon sinks, Taiwan should develop novel CDRs such as bioenergy with carbon capture and storage, afforestation, reforestation, biochar, seaweed cultivation, and ocean alkalinity enhancement, to reach carbon neutrality by 2050.

4. **Xu, C., Goranov, A.I., Kaplan, D.I., Lin, P., Yeager, C.M., Patterson, N., Jiang, H., Ware, S., Hatcher, P.G., Santschi, P.H. 2024. Molecular features of uranium-binding natural organic matter in a DOE site using ultrahigh resolution mass spectrometry. STOTEN 174867.**

Abstract: Tims Branch riparian wetland located in South Carolina, USA has immobilized 94 % of the U released >50 years ago from a nuclear fuel fabrication facility. Sediment organic matter (OM) has been shown to play an important role in immobilizing U. Yet, uranium-OM-mineral interactions at the molecular scale have never been investigated at ambient concentrations. The objectives of this study were to extract, purify, and concentrate U-bound sediment OM along the stream water pathway and perform molecular characterization using Fourier transform ion cyclotron resonance mass spectrometry (FTICRMS). Out of 9614 identified formulas, 715 contained U. These U-containing formulas were enriched with Fe, N, and/or S compared to the total OM. Lignin-like and protein-like molecules accounted for 40 % and 19 % of the U-containing formulas, respectively. Phosphorus-containing formulas were found to exert an insignificant influence on complexing U. U-containing formulas in the ‘mobile’ (groundwater extractable) OM fraction had lower (reduced) nominal oxidation states of carbon (NOSC); and less aromatic moieties than OM recovered from the ‘immobile’ (sodium pyrophosphate extractable) OM fraction. U-containing formulas in the redox interfacial zones (stream banks) compared to those in nearby up-slope zones tended to have smaller molecular weights; lower NOSC; higher contents of COO and/or CONO functional groups; and higher abundance of Fe-containing formulas. Fe was present in 38 % of the U-containing formulas but only 20 % of the total OM formulas. It is postulated that Fe played an important role in stabilizing the structure of sedimentary OM, especially U-containing compounds. The identification for the first time of hundreds of Fe-UOM formulas demonstrates the complexity of such system is much greater than commonly believed and numerically predicting U binding behavior in OM-rich systems may require greater use of statistical or artificial intelligence approaches rather than deterministic approaches limited to measuring metal complexation with well-defined individual analogue organic ligands.

5. **Santschi, P.H., Xu, C., Lin, P., Yeager, C.M., Hazenberg, P., Kaplan, D.I. 2024. Hydrological controls of a riparian wetland based on stable isotope data and model simulations. Isotopes in Environmental and Health Studies.**

Abstract: Isotopic evidence of groundwater and stream water is frequently used to investigate water exchanges with groundwater. Monthly sampling of rain, stream water, and groundwater was conducted at Tims Branch watershed in South Carolina for the oxygen and hydrogen stable isotope (δ^2H and $\delta^{18}O$) measurement, as well as pH and oxidation–reduction potential (ORP). Together with a mass balance perspective, it was determined that it takes a few weeks to one month for groundwater in the hyporheic zone to fully exchange with stream water. From hydrodynamic modelling, we show that substantial (up to 70 %) groundwater exchange occurs at gaining and losing sites. Groundwater exfiltration, i.e. inflow into stream water, contributes up to 4 % to stream water, with the remainder from upstream exfiltration. A 2–4 % per day renewal rate of adjacent groundwater would indirectly indicate a groundwater residence time in the order of half a month to a full month (assuming either a well-mixed case or large dispersion rate in pulse flow case), in agreement with a greatly reduced variability of δ^2H and $\delta^{18}O$ of groundwater compared to stream water and rain. This reduced variability of stable isotope signal from groundwater confirms our hypothesis that riparian groundwater mixing at Tims Branch is more of a mixed type rather than a pulse flow type. A monthly time scale is sufficient for groundwater to become anoxic at exit points into stream water resulting in the episodic production of natural organic matter- and iron-rich flocs upon oxidation.

Unusual Sabatier Principle on High Entropy Alloy Catalysts for Hydrogen Evolution Reactions

by Qing Jiang, Member EUAS

Short Biography

Qing Jiang is a Professor of the School of Materials Science and Engineering, Jilin University since 1992. He received his BSc and MSc in Materials Science from Jilin University of Technology (merged into Jilin University in 2000) in 1982 and 1984, respectively, and PhD in Chemistry from University of Stuttgart, Germany in 1990.

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 also a Fellow of The Institute of Physics (U.K.), and members of the editor board of several academic journals.

His current research interests include synthesis of nanomaterials as well as their applications in catalysis, energy storage and conversion (fuel cell, batteries, supercapacitors, and electrocatalysis), with focus on kinetics aspects of mass transfer and chemical reaction. He has published more than 800 papers in peer-reviewed journals, including Nat. Nanotechnol., Nat. Chem., Nat. Commun., Sci. Adv., Joule, Chem, Matter, etc. His publications have been cited more than 39,000 times with H-index = 100 (Web of Science).

In 2024, he authored and coauthored 40 papers and several representative ones with their abstracts are listed below:

1. Zhi Wen Chen, Jian Li, Pengfei Ou, Jianan Erick Huang, Zi Wen, LiXin Chen, Xue Yao, GuangMing Cai, Chun Cheng Yang*, Chandra Veer Singh*, Qing Jiang*, Unusual Sabatier principle on high entropy alloy catalysts for hydrogen evolution reactions, Nat. Commun., 2024, 15, 359.

Abstract

The Sabatier principle is widely explored in heterogeneous catalysis, graphically depicted in volcano plots. The most desirable activity is located at the peak of the volcano, and further advances in activity past this optimum are

possible by designing a catalyst that circumvents the limitation entailed by the Sabatier principle. Herein, by density functional theory calculations, we discovered an unusual Sabatier principle on high entropy alloy (HEA) surface, distinguishing the "just right" ($\Delta G_{H^*} = 0$ eV) in the Sabatier principle of hydrogen evolution reaction (HER). A new descriptor was proposed to design HEA catalysts for HER. As a proof-of-concept, the synthesized PtFeCoNiCu HEA catalyst endows a high catalytic performance for HER with an overpotential of 10.8 mV at −10 mA cm^{-2} and 4.6 times higher intrinsic activity over the state-of-the-art Pt/C. Moreover, the unusual Sabatier principle on HEA catalysts can be extended to other catalytic reactions.

2. Hang Shi, Tian-Yi Dai, Xin-Ying Sun, Zhi-Lan Zhou, Shu-Pei Zeng, Tong-Hui Wang, Gao-Feng Han, Zi Wen, Qian-Rong Fang, Xing-You Lang*, Qing Jiang*, Dual-Intermetallic Heterostructure on Hierarchical Nanoporous Metal for Highly Efficient Alkaline Hydrogen Electrocatalysis, Adv. Mater. 2024, 36, 2406711.

Abstract

Developing robust nonprecious-metal electrocatalysts with high activity towards sluggish oxygen-evolution reaction is paramount for large-scale hydrogen production via electrochemical water splitting. Here we report that self-supported laminate composite electrodes composed of alternating nanoporous bimetallic iron-cobalt alloy/oxyhydroxide and cerium oxynitride ($FeCo/CeO_{2-x}N_x$) heterolamellas hold great promise as highly efficient electrocatalysts for alkaline oxygen-evolution reaction. By virtue of three-dimensional nanoporous architecture to offer abundant and accessible electroactive $CoFeOOH/CeO_{2-x}N_x$ heterostructure interfaces through facilitating electron transfer and mass transport, nanoporous $FeCo/CeO_{2-x}N_x$ composite electrodes exhibit superior oxygen-evolution electrocatalysis in 1 M KOH, with ultralow Tafel slope of ~33 mV dec^{-1}. At overpotential of as low as 360 mV, they reach >3900 mA cm^{-2} and retain exceptional stability at ~1900 mA cm^{-2} for >1000 h, outperforming commercial RuO_2 and some representative oxygen-evolution-reaction catalysts recently reported. These electrochemical properties make them attractive candidates as oxygen-evolution-reaction electrocatalysts in electrolysis of water for large-scale hydrogen generation.

3. Huan Meng, Qing Ran, Tian-Yi Dai, Jian-Hui Jia, Jie Liu, Hang Shi, Gao-Feng Han, Tong-Hui Wang, Zi Wen, Xing-You Lang*, Qing Jiang*, Lamellar Nanoporous Metal/Intermetallic Compound Heterostructure Regulating Dendrite-Free Zinc Electrodeposition for Wide-Temperature Aqueous Zinc-Ion Battery, Adv. Mater. 2024, 36, 2403803.

Abstract

Aqueous zinc-ion batteries are attractive post-lithium battery technologies for grid-scale energy storage because of their inherent safety, low cost and high theoretical capacity. However, their practical implementation in wide-temperature surroundings persistently confronts irregular zinc electrodeposits and parasitic side reactions on metal anode, which leads to poor rechargeability, low Coulombic efficiency and short lifespan. Here, this work reports lamellar nanoporous Cu/Al_2Cu heterostructure electrode as a promising anode host material to regulate high-efficiency and dendrite-free zinc electrodeposition and stripping for wide-temperatures aqueous zinc-ion batteries. In this unique electrode, the interconnective Cu/Al_2Cu heterostructure ligaments not only facilitate fast electron transfer but work as highly zincophilic sites for zinc nucleation and deposition by virtue of local galvanic couples while the interpenetrative lamellar channels serving as mass transport pathways. As a result, it exhibits exceptional zinc plating/stripping behaviors in aqueous hybrid electrolyte of diethylene glycol dimethyl ether and zinc trifluoromethanesulfonate at wide temperatures ranging from 25 to −30 °C, with ultralow voltage polarizations at various current densities and ultralong lifespan of >4000 h. The outstanding electrochemical properties enlist full cell of zinc-ion batteries constructed with nanoporous Cu/Al_2Cu and $Zn_xV_2O_5$/C to maintain high capacity and excellent stability for >5000 cycles at 25 and −30 °C.

4. Hong-Bo Chen, Huan Meng, Tong-Rui Zhang, Qing Ran, Jie Liu, Hang Shi, Gao-Feng Han, Tong-Hui Wang*, Zi Wen, Xing-You Lang*, Qing Jiang*, Dynamic Molecular Interphases Regulated by Trace Dual Electrolyte Additives for Ultralong-Lifespan and Dendrite-Free Zinc Metal Anode, Angew. Chem. Int. Ed. 2024, 63, e202402327

Abstract

Hybrid aqueous electrolyte of $ZnSO_4$ with trace dual electrolyte additives of D-mannose and sodium lignosulfonate enables ultralong-lifespan and dendrite-free Zn metal anode by virtue of D-mannose and lignosulfonate species alternately and reversibly adsorb on Zn surface to form dynamical molecular interphases and enter Zn^{2+} solvation sheath to boost de-solvation kinetics. Zn anode in such dual-additive electrolyte exhibits exceptional

stability for >6400 hours.

5. Tian-Yi Dai, Hang Shi, Tong-Hui Wang*, Xing-You Lang*, Qing Jiang*, Achieving a Thermodynamic Self-Regulation Dynamic Adsorption Mechanism for Ammonia Synthesis through Selective Orbital Coupling, Angew. Chem. Int. Ed. 2024, e202418035.

Abstract

With the continuous pursuing on the improvement of catalytic activity, a catalyst performed exceeding catalytic volcano plots is desired, while it is impeded by the adsorption-energy scaling relations of reaction intermediates. Numerous efforts have been focused on optimizing the initial and final intermediates to circumvent the scaling relations for an improved performance. For a step forward, simultaneously optimizing all intermediates is essential to explore the theoretical maximum of catalytic activity. Herein, we proposed a dynamic adsorption mechanism (DAM) to independently regulate the adsorption configurations of all intermediates of electrochemical nitrogen reduction reaction (NRR). To demonstrate the DAM, a multi-site $NbNi_3$ intermetallic is developed, which enables suitable adsorption energies of different intermediates via modulating orbital coupling mechanisms. As a result, $NbNi_3$ achieves an ultra-low limiting potential of NRR of −0.11V *vs*. reversible hydrogen electrode (RHE). Strikingly, the theoretical result is confirmed by a proof-of-concept experiment, wherein the nanoporous $NbNi_3$ electrode exhibits a remarkable NH_3 yield rate of 25.89 $\mu g\, h^{-1}\, cm^{-2}$ with the Faradaic efficiency of 33.15 % at −0.25 V *vs*. RHE. Overall, this work brings out a new strategy to avoid the scaling relations, and opens up a promising avenue toward high-efficiency NRR catalysts.

Incorporating Catalytic Units into Nanomaterials: Rational Design of Multipurpose Catalysts for CO2 Valorization

by Liang-Nian He, Member EUAS

Short Biography

Prof. Liang-Nian He is a renowned Chinese chemist known for his exceptional contributions to green chemistry, catalysis, renewable energy chemistry, and CO2 chemistry. His groundbreaking work focuses on the catalytic conversion of CO2 into fuels and valuable chemicals, aiming to promote sustainability through carbon-neutral processes. Prof. He has an extensive academic and professional background, having worked in prestigious international institutions and published over 300 research papers. His research has garnered significant recognition, placing him among the most cited researchers in the field. He is a Professor of Chemistry at Nankai University and holds several prestigious fellowships, including being a Fellow of the Royal Society of Chemistry. Prof. He's work has not only made theoretical contributions but also developed industrially applicable CO2 conversion technologies.

Prof. Liang-Nian He obtained his doctorate in Chemistry from Nankai University in 1996. After completing his Ph.D., he worked as a postdoctoral associate at Wuhan University (1996-1998), collaborating with renowned chemist Prof. Ren-Xi Zhuo. During his academic journey, Prof. He was awarded international fellowships, including those from the AIST (National Institute of Advanced Science and Technology, Japan) from 2002-2003 and the NEDO (New Energy and Development Organization, Japan) fellowship from 1999-2002. These fellowships helped him further deepen his expertise in chemistry and catalysis. His formal education, combined with international postdoctoral training, laid a strong foundation for his future research endeavors.

Prof. Liang-Nian He has an impressive professional trajectory in both academic and international research environments. Currently, he is a Professor of Chemistry at Nankai University, one of China's top research institutions. In addition to his academic role, Prof. He has contributed significantly to international scientific communities, having held prestigious fellowships such as the CSIRO Distinguished Visiting Professor at the Commonwealth Scientific and Industrial Research Organization in Australia in 2019. He has also been a recipient of the "Chutian Scholarship" Distinguished Professor award and has served in various capacities, including editorial roles for scientific publications and as an invited speaker at over 80 international conferences, further showcasing his influence in the global scientific arena. He is on the editorial board of a dozen of international scientific journals including "Green Chemistry and Sustainable Technology" (Springer) Series Editor, Frontier in Chemistry, Journal of CO2 Utilization (Elsevier), ChemistryOpen (Wiley), Current Opinion in Green and Sustainable Chemistry (Elsevier), Mini-review in Organic Chemistry, Green Chemical Engineering, ChemCatChem (Wiley), Carbon and Hydrogen (Wiley), as well as successfully organizing conferences and symposia on CO2 chemistry/CO2 capture and utilization.

Prof. Liang-Nian He's research focuses on the fields of green chemistry, catalysis, renewable energy chemistry, and CO2 chemistry. His work emphasizes the catalytic activation and transformation of CO2 into valuable chemicals and fuels, contributing to

environmental sustainability and carbon-neutral technologies. He explores the integration of CO2 capture and conversion processes, aiming to close the carbon cycle through renewable energy-driven processes. Prof. He's research also includes the development of novel catalytic materials and processes for biomass conversion and desulfurization technologies. His innovative work has far-reaching applications, addressing critical challenges in energy and environmental chemistry.

Prof. Liang-Nian He has received numerous prestigious awards and honors in recognition of his groundbreaking work in chemistry. He became a Fellow of the Royal Society of Chemistry in 2011, cementing his status as a leading figure in the field. In 2014, he was named one of the Most Cited Chinese Researchers by Elsevier, a distinction he held through 2024. Additionally, Prof. He was recognized as one of the top 1% highly cited authors in RSC journals from 2014-2020. He has also been the recipient of the Advancement of Science and Technology Award from the PLA in 2017, and the Nature Science Award of Tianjin in 2015. These accolades highlight the global recognition of his contributions to science, particularly in the areas of catalysis and CO2 chemistry.

Recent Publications

1. **Li-Qi Qiu, Hong-Ru Li,* and Liang-Nian He*, Incorporating Catalytic Units into Nanomaterials: Rational Design of Multipurpose Catalysts for CO_2 Valorization,** ***Acc. Chem. Res.*** 2023**,** ***56*** **(16), 2225-2240.**

Abstract

CO_2 conversion to valuable chemicals is effective at reducing CO_2 emissions. We previously proposed valorization strategies and developed efficient catalysts to address thermodynamic stability and kinetic inertness issues related to CO_2 conversion. Earlier, we developed molecular capture reagents and catalysts to integrate CO_2 capture and conversion, i.e., in situ transformation. Based on the mechanistic understanding of CO_2 capture, activation, and transformation at a molecular level, we set out to develop heterogeneous catalysts by incorporating catalytic units into nanomaterials via the immobilization of active molecular catalysts onto nanomaterials and designing nanomaterials with intrinsic catalytic sites. In thermocatalytic CO_2 conversion, carbonaceous and metal−organic framework (MOF)- based catalysts were developed for nonreductive and reductive CO_2 conversion. Novel Cu- and Zn-based MOFs and carbon-supported Cu catalysts were prepared and successfully applied to the cycloaddition, carboxylation, and carboxylative cyclization reactions with CO_2, generating cyclic carbonates, carboxyl acids, and oxazolidinones as respective target products. Reductive conversion of CO_2, especially reductive functionalization with CO_2, is a promising transformation strategy to produce valuable chemicals, alleviating chemical production that relies on petrochemistry. We explored the hierarchical reductive functionalization of CO_2 using organocatalysts and

proposed strategies to regulate the CO_2 reduction level, triggering heterogeneous catalyst investigation. Introducing multiple active sites into nanomaterials opens possibilities to develop novel CO_2 transformation strategies. CO_2 capture and in situ conversion were realized with an N-doped carbon-supported Zn complex and MOF materials as CO_2 adsorbents and catalysts. These nanomaterial-based catalysts feature high stability and excellent efficiency and act as shape-selective catalysts in some cases due to their unique pore structure. Nanomaterial-based catalysts are also appealing candidates for photocatalytic CO_2 reduction (PCO2RR) and electrocatalytic CO_2 reduction (ECO_2RR), so we developed a series of hybrid photo-/electrocatalysts by incorporating active metal complexes into different matrixes such as porous organic polymers (POPs), metal−organic layers (MOLs), micelles, and conducting polymers. By introducing Re-bipyridine and Fe-porphyrin complexes into POPs and regulating the structure of the polymer chain, catalyst stability and efficiency increased in PCO_2RR. PCO_2RR in aqueous solution was realized by designing the Re-bipyridine-containing amphiphilic polymer to form micelles in aqueous solution and act as nanoreactors. We prepared MOLs with two different metallic centers, i.e., the Ni-bipyridine site and Ni-O node, to improve the efficiency for PCO_2RR due to the synergistic effect of these metal centers. Sulfylphenoxy-decorated cobalt phthalocyanine (CoPc) cross-linked polypyrrole was prepared and used as a cathode, achieving the electrocatalytic transformation of diluted CO_2 benefiting from the CO_2 adsorption capability of polypyrrole. We fabricated immobilized 4-(t-butyl)-phenoxy cobalt phthalocyanine and Bi-MOF as cathodes to promote the paired electrolysis of CO_2 and 5-hydroxymethylfurfural (HMF) and obtained CO2 reductive products and 2,5-furandicarboxylic acid (FDCA) efficiently.

2. **Li-Qi Qiu, Xiang-yang Yao, Yong-Kang Zhang, Hong-Ru Li*, Liang-Nian He*, Advancements and Challenges in Reductive Conversion of Carbon Dioxide via Thermo-/Photocatalysis .** ***J. Org. Chem.*** 2023**,** ***88*** **(8), 4942–4964.**

Abstract

Carbon dioxide (CO_2) is the major greenhouse gas and also an abundant and renewable carbon resource. Therefore, its chemical conversion and utilization are of great attraction for sustainable development. Especially, reductive conversion of CO_2 with energy input has become a current hotspot due to its ability to access fuels and various important chemicals. Nowadays, the controllable CO_2 hydrogenation to formic acid and alcohols using sustainable H_2 resources has been regarded as an appealing solution to hydrogen storage and CO_2 accumulation. In addition, photocatalytic CO_2 reduction to CO also

provides a potential way to utilize this greenhouse gas efficiently. Besides direct CO_2 hydrogenation, CO2 reductive functionalization integrates CO2 reduction with subsequent C–X (X = N, S, C, O) bond formation and indirect transformation strategies, enlarging the diverse products derived from CO_2 and promoting CO_2 reductive conversion into a new stage. In this Perspective, the progress and challenges of CO_2 reductive conversion, including hydrogenation, reductive functionalization, photocatalytic reduction, and photocatalytic reductive functionalization are summarized and discussed along with the key issues and future trends/directions in this field. We hope this Perspective can evoke intense interest and inspire much innovation in the promise of CO_2 valorization.

3. **Fang-Yu Ren, Kaihong Chen, Li-Qi Qiu, Jin-Mei Chen, Donald J. Darensbourg*, Liang-Nian He*, Amphiphilic Polycarbonate Micellar Rhenium Catalysts for Efficient Photocatalytic CO_2 Reduction in Aqueous Media.** ***Angew. Chem. Int. Ed.*** 2022**, *61*, e202200751.**

Abstract
A triblock amphiphilic polymer derived from the copolymerization of CO_2 and epoxides containing a bipyridine rhenium complex in its backbone is shown to effectively catalyze the visible-light-driven reduction of CO_2 to CO. This polymer provides uniformly spherical micelles in aqueous solution, where the metal catalyst is sequestered in the hydrophobic portion of the nanostructured micelle. CO_2 to CO reduction occurs in an efficient visible-light-driven process in aqueous media with turnover numbers up to 110 (> 99% selectivity) in the absence of a photosensitizer, which is a 37-fold enhancement over the corresponding molecular rhenium catalyst in organic solvent. Notably, the amphiphilic polycarbonate micelle rhenium catalyst suppresses H_2 generation, presumably by preventing deactivation of the active catalytic center by water.

4. **Zhi-Wen Yang, Jin-Mei Chen, Li-Qi Qiu, Wen-Jun Xie, Liang-Nian He*, Molecular Engineering of Metal Complexes for Electrocatalytic Carbon Dioxide Reducton: From Adjustment of Intrinsic Activity to Molecular Immobilization.** ***Angew. Chem. Int. Ed.*** 2022**, *61*, e202205301.**

Abstract
Electrocatalytic CO_2 reduction reaction (ECO_2RR) is one promising method for storing intermittent clean energy in the chemical bonds and producing fuels. Among various kinds of catalysts for ECO_2RR, molecular metal

complexes with well-defined structures, thus offer convenient approaches to perform rational designing, investigation about the structure-reactivity relationship and mechanistic studies. In this review, we summarize the molecular engineering of several N-based metal complexes including Re/Mn bipyridine compounds and metal macrocycles, concluding the general modification strategies to devise novel molecular catalysts with high intrinsic activity. Through physical adsorption, covalent linking and forming periodic backbone, these active molecules could be heterogenized into immobilized catalysts with more practical prospect. In the end, significant challenges and opportunities based on molecular catalysts are put forward.

5. **Mei-Yan Wang, Xin Jin, Xiao-Fei Wang, Shu-Mei Xia, Yue Wang, Shou-Ying Huang, Ying Li, Liang-Nian He*, Xinbin Ma*, Copper-Catalyzed and Proton-Directed Selective Hydroxymethylation of Alkynes with CO2, Angew. Chem. Int. Ed., 2021, 60, 3984-3988.**

Abstract
An intriguing strategy for copper-catalyzed hydroxymethylation of alkynes with CO2 and hydrosilane was developed. Switched on/off a proton source, e.g. tBuOH, direct hydroxymethylation and reductive hydroxymethylation could be triggered selectively, delivering a series of allylic alcohols and homobenzylic alcohols respectively, with high levels of Z/E, regio- and enantioselectivity. Such a selective synthesis is attributed to the differences in response of vinylcopper intermediate to proton and CO_2. The protonation of vinylcopper species is demonstrated to be prior to hydroxymethylation, thus allowing a diversion from direct alkyne hydroxymethylation to reductive hydroxymethylation in the presence of suitable proton.

6. **Chun-Shuai Cao, Shu-Mei Xia, Zhen-Jun Song, Hang Xu, Ying Shi, Liang-Nian He*, Peng Cheng, and Bin Zhao* Highly Efficient Conversion and Reaction Mechanism of Propargylic Amines and CO2 Catalyzed by Eco-Friendly Noble-Metal-Free [Zn116] Nanocages. Angew. Chem. Int. Ed., 2020, 59, 22, 8586-8593**

Abstract
The reaction of propargylic amines and CO2 can provide high-value-added chemical products. However, most of catalysts in such reactions employ noble metals to obtain high yield, and it is important to seek eco-friendly noble-metal-free MOFs catalysts. Here, a giant and lantern-like $[Zn_{116}]$ nanocage in zinc-tetrazole 3D framework
$[Zn_{22}(Trz)_8(OH)_{12}(H_2O)_9\cdot 8\,H_2O]n$ Trz=$(C_4N_{12}O)_4$ was obtained and structurally characterized. It consists of six $[Zn_{14}O_{21}]$ clusters and eight

[Zn_4O_4] clusters. To our knowledge, this is the highest-nuclearity nanocages constructed by Zn-clusters as building blocks to date. Importantly, catalytic investigations reveal that 1 can efficiently catalyze the cycloaddition of propargylic amines with CO_2, exclusively affording various 2-oxazolidinones under mild conditions. It is the first eco-friendly noble-metal-free MOFs catalyst for the cyclization of propargylic amines with CO_2. DFT calculations uncover that ZnII ions can efficiently activate both C≡C bonds of propargylic amines and CO_2 by coordination interaction. NMR and FTIR spectroscopy further prove that Zn-clusters play an important role in activating C≡C bonds of propargylic amines. Furthermore, the electronic properties of related reactants, intermediates and products can help to understand the basic reaction mechanism and crucial role of the catalyst.

Damage and Fracture in Metals: Experiments, Modeling and Numerical Analysis

by Michael Brünig, Member EUAS

Short Biography

Michael Brünig is currently Professor for Mechanics in the Faculty of Civil Engineering and Environmental Sciences at the University of the Bundeswehr Munich in Germany. He is a member of the International Association of Applied Mathematics and Mechanics, the European Mechanics Society, the German Association for Computational Mechanics and the EU Academy of Sciences.

He received his Diplom degree in civil engineering at the University of Hannover in 1985. From 1985 to 1989 he worked at the Ruhr-University Bochum in a project on roller-straightening of rails. 1989 he received his Doktor degree from the Faculty of Civil Engineering in Bochum. From 1990 to 2010 he was senior researcher and lecturer at the University of Dortmund working in the fields of plasticity, damage and fracture of engineering materials like metals, concrete and polymers. In Dortmund he received his Habilitation degree in 1998. In 2010 he became full professor at the University of the Bundeswehr Munich where he was Vice Dean from 2018 to 2020 and Dean of the Faculty of Civil Engineering and Environmental Sciences from 2020 to 2022. In addition, he was visiting professor at the University of São Paulo, Brazil.

Michael Brünig is Technical Editor of the international journal Experimental Mechanics, Regional Editor of Recent Patents on Mechanical Engineering as well as member of the Editorial Boards of 10 other journals including International Journal of Plasticity and International Journal of Damage Mechanics.

Damage and Fracture in Metals

1. Experiments

During the last decades many high-quality metals and alloys have been developed to fulfill industrial demands like improvement of cost efficiency, reduction in energy consumption and increase of safety and lifetime. During loading of structural elements often damage occurs on the micro-scale leading to ductile fracture on the macro-level which can cause the end of life of structures. The analysis of failure mechanisms requires a sophisticated experimental program to detect stress-state-dependent damage and fracture processes.

In particular, uniaxial tension tests with unnotched and differently notched specimens have been performed to identify basic material parameters as well as to investigate the effect of the stress state on inelastic deformation behavior as well as on damage and failure mechanisms [1,2]. Analysis of shear-dominated stress states is based on uniaxially loaded specimens with special geometries undergoing shear deformation [2]. Since experiments with uniaxially loaded specimens only cover a small range of stress states appearing in practical applications, an extended testing program with biaxially loaded cruciform specimens has been developed [3,4]. Alternative geometries of the biaxially loaded cruciform specimens have been proposed to analyze the influence of different proportional, non-proportional and reverse load paths as well as of a wide range of stress states on inelastic deformation as well as damage and fracture behavior in ductile metals [5-8]. Optimization of these geometries has been performed to receive the required stress states during the loading process [9]. During the experiments respective loads and corresponding displacements are recorded by a biaxial machine. In addition, 3D strain fields in critical regions of the specimens are monitored by digital image correlation using eight cameras and a lighting system [10]. After the tests fracture surfaces of the specimens are analyzed by scanning electron microscopy revealing stress-state- and loading-direction-dependent fracture modes [6-8,10].

2. Modeling

Based on the experimental observations and results a phenomenological continuum model was developed to predict the deformation behavior as well as the stress state and damage distribution in metal structures [11]. This continuum-mechanics-based framework uses the introduction of damaged and corresponding undamaged configurations. A yield criterion predicts onset of plastic yielding and a flow rule describes the evolution of irreversible plastic strains caused by crystallographic movements on the micro-scale. In addition, a damage criterion models onset of damage and the formation of macroscopic damage strains is governed by a damage rule. These macroscopic damage strains are caused by the evolution of micro-pores and micro-shear-cracks originated from different loadings. However, it is not possible to detect all relevant damage processes on the micro-scale using experimental techniques. Therefore, bridging the scales additional numerical calculations on the micro-level considering pre-damaged representative volume elements have been performed to reveal details of damage and fracture mechanisms on the micro-scale and their effect on the macroscopic deformation behavior. This leads to modifications in the continuum damage model [12]. Furthermore, non-proportional and reverse loading paths demand changes in the yield and

damage conditions with complex evolution equations [13]. Moreover, the forming process for thin sheets leads to anisotropies in ductile metals caused by internal changes in the crystallographic texture which have to be taken into account in appropriate material models. This leads to a generalization of the yield criterion and the damage condition with functions depending on the direction of loading with respect to the principal axes of anisotropy [14,15].

3. Numerical Analysis

Numerical analysis on the micro-level is used to detect damage processes under different stress states and to develop corresponding evolution equations for macroscopic variables [12,16]. Void-containing representative volume elements are three-dimensionally loaded with different load ratios to cover a wide range of stress states. Analysis of the anisotropic deformation of the voids and the macroscopic stress state allow formulation of equations modeling the macroscopic stress-strain behavior and the proposition of damage equations.

On the other hand, numerical analysis on the macro-level is used to validate the continuum damage model [3,4,6,7,13]. The behavior of uniaxially and biaxially loaded specimens is numerically analyzed. Numerically predicted load-displacement curves are compared with experimental ones. In critical zones of the specimens, where damage and fracture are expected to occur, strain fields monitored by digital image correlation are compared with the numerically obtained ones. In addition, from the numerical analysis stress fields are obtained allowing prediction of the stress-state-dependent damage processes on the micro-level. These can be compared with pictures from scanning electron microscopy of the fractured surfaces showing various micro-defects and fracture modes.

After validation of the material model by comparison of numerical results and experimental data, the finite element program based on the continuum framework can be used to predict inelastic deformation behavior and amount of damage in structural components after complex loading conditions. This is relevant for the optimization of metal forming processes as well as in the prediction of service and lifetime of engineering structures.

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Marine Biology: Comparative Ecology of Planet Ocean

by Roberto Danovaro, Member EUAS

Short Biography

Roberto Danovaro was the Director of the Department of Marine Sciences (2004-2010), Director of the Department of Life and Environmental Sciences (2011-2014) and Pro-Rector (Delegated to the Research) (2010-2013). President of the Italian Society of Ecology (2011-2013), and of the Italian Society of Limnology and Oceanography (2008-2011). Roberto Danovaro received several Awards, including the World Prize BMC Biology (2010), the Award of French Society of Oceanography (2011), and the ENI Award Protection of the Environment (2013). Nominated in 2013 (renewed 2018-2022) by the Ministry of Education University and Research, President of the Stazione Zoologica Anton Dohrn (National Institute of Marine Biology Ecology and Biotechnology). In 2020 Roberto Danovaro has been recognized by ExpertScape as the top World Scientist in the Category "Ocean and Seas" for the decade 2010-2020. Roberto Danovaro was member of the EU Network of Excellence: MARBEF (Marine Biodiversity and ecosystem functioning), EUROCEANS (European Research on Ocean Ecosystems under Anthropogenic and Natural forcing), and CAREX (European Life in Extreme Environments). He participated in more than 25 international research projects (either EU or ESF). Roberto Danovaro was the president of the Scientific Council of WWF Italy, and member of the Steering Board of OECD (Fostering Innovation in Ocean Economy), member of the Scientific Council of several research institutions and panels (IUCN, UNEP, EU), and coordinator of several EU and international programs. Roberto Danovaro was President of the Italian Society of Ecology (2011-2013), and of the Italian Society of Limnology and Oceanography (2008-2011) and the European Federation of Scientific Technological Societies (2008-2012). Roberto Danovaro is a member of the Academia Europaea (European Science Academy), of the EU Academy of Sciences, of the Society for Ecosystem Restoration (SER) and of the Deep-Sea Biology Society (DSBS). His scientometric: H index 107, 550+ articles with IF (WoS), ca 42,000 citations. He has published as leading Author, last or corresponding Author of several articles published in Nature, Science, Science Advances, Nature Communications, Nature Microbiol Reviews, PNAS, Nature Ecology Evolution, Trends Ecology Evolution on topics relative to the marine ecosystems biodiversity, ocean health, impact of climate change on seas and oceans and marine ecosystem restoration. He is Editor in Chief of the journals Marine Ecology (Wiley) and Chemistry and Ecology (Taylor & Francis.

Selected Publications 2024

BOOK: Marine Biology: Comparative Ecology of Planet Ocean
Roberto Danovaro, Paul Snelgrove
Publisher: John Wiley & Sons

MARINE BIOLOGY Marine Biology: Comparative Ecology of Planet Ocean provides a learning tool to those who love the ocean to help them understand and learn about the life that populates it, the extraordinary adaptations of marine organisms to their environment, and the spectacular variety of marine life forms that inhabit the many marine habitats and contribute to the life support system of Planet Ocean. The book introduces marine biology by seeing the ocean through the eyes of its inhabitants, describing the properties of sea water, the surface waters and its currents, and the characteristics of the seabed according to how marine organisms perceive, exploit, and shape them. This book explains to the reader and those who love the ocean not only how to recognize the most common marine organisms and habitats, from the coast to great depths, but it also explains their complex life cycles and the environmental factors controlling their distribution, reproduction, and growth. Finally, the book evaluates the role that living biota play in how different marine ecosystems function to understand better their characteristics, peculiarities, and threats. This book offers an up-to-date and comprehensive text on the study of marine biology, presenting insights into the methodologies scientists have adopted for the study of marine ecosystems. It also includes chapters about human impacts on marine biodiversity, from overfishing to climate change, from pollution (including microplastics) to alien-species invasions, from conservation of marine resources to the restoration of degraded marine habitats. pp 698.

Making eco-sustainable floating offshore wind farms: Siting, mitigations, and compensations

Roberto Danovaro, Silvia Bianchelli, Paola Brambilla, Gaia Brussa, Cinzia Corinaldesi, Adriana Del Borghi, Antonio Dell'Anno, Simonetta Fraschetti, Silvestro Greco, Mario Grosso, Ettore Nepote, Lucia Rigamonti, Ferdinando Boero. ***Renewable and Sustainable Energy Reviews (2024), 197, 114386.***

Floating Offshore Wind Farms (FOWFs) are the most promising renewable energy resource. Floating turbines are installed at progressively increasing water depths, interacting with offshore and deep-sea ecosystems. Thus, specific criteria to enable a sound and accurate Environmental Impact Assessment (EIA) are required. The still limited understanding of the impacts of FOWFs, and the concerns for the conflicts in the use of maritime space (e.g., fisheries), might lead to a more precautionary approach and constrain their development. Here we describe the characteristics of the deep habitats potentially impacted and identify a set of

comprehensive and standardized criteria, response variables and approaches for a reliable EIA based on an Ecosystem-based approach. These analyses will support an appropriate design and site prioritization to respect the “Do No Significant Harm" principle. Considering the wide heterogeneity among habitats and geographic regions, we examined the potential interactions of FOWFs with i) Vulnerable Marine Ecosystems; ii) critical habitats; iii) migratory routes of large marine vertebrates; iv) habitat-forming species, benthic/pelagic organisms, v) migratory routes of birds/chiropters; vi) other human uses leading to cumulative/synergistic effects and any other potential interference. We identified mitigation and compensation measures and explored the potential of wind-farm areas as “Other Effective Conservation Measures” to support sustainable fisheries and passive restoration. Adequate sitting, EIA and systematic monitoring can minimize FOWFs’ environmental interactions, with final negligible, or even positive effects on marine ecosystems. Standardized criteria could significantly reduce the bottlenecks in permitting while offering a strategic vision for the sustainable use of maritime space.

Microbes as marine habitat formers and ecosystem engineers

Roberto Danovaro, Lisa A. Levin, Ginevra Fanelli, Lorenzo Scenna & Cinzia Corinaldesi *Nature Ecology & Evolution (2024), 8, 1407-1419.*

Despite their small individual size, marine prokaryotic and eukaryotic microbes can form large 3D structures and complex habitats. These habitats contribute to seafloor heterogeneity, facilitating colonization by animals and protists. They also provide food and refuge for a variety of species and promote novel ecological interactions. Here we illustrate the role of microbes as ecosystem engineers and propose a classification based on five types of habitats: microbial mats, microbial forests, microbial-mineralized habitats, microbial outcrops and microbial nodules. We also describe the metabolic processes of microbial habitat formers and their ecological roles, highlighting current gaps in knowledge. Their biogeography indicates that these habitats are widespread in all oceans and are continuously being discovered across latitudes and depths. These habitats are also expected to expand under future global change owing to their ability to exploit extreme environmental conditions. Given their high ecological relevance and their role in supporting endemic species and high biodiversity levels, microbial habitats should be included in future spatial planning, conservation and management measures.

Resistance to freezing conditions of endemic Antarctic polychaetes is enhanced by cryoprotective proteins produced by their microbiome

Emanuela Buschi, Antonio Dell’Anno, Michael Tangherlini, Marco Candela, Simone Rampelli, Silvia Turroni, Giorgia Palladino, Erika Esposito, Marco Lo Martire, Cinzia Corinaldesi

The microbiome plays a key role in the health of all metazoans. Whether and how the microbiome favors the adaptation processes of organisms to extreme conditions, such as those of Antarctica, which are incompatible with most metazoans, is still unknown. We investigated the microbiome of three endemic and widespread species of Antarctic polychaetes: Leitoscoloplos geminus, Aphelochaeta palmeri, and Aglaophamus trissophyllus. We report here that these invertebrates contain a stable bacterial core dominated by Meiothermus and Anoxybacillus, equipped with a versatile genetic makeup and a unique portfolio of proteins useful for coping with extremely cold conditions as revealed by pangenomic and metaproteomic analyses. The close phylosymbiosis between Meiothermus and Anoxybacillus and these Antarctic polychaetes indicates a connection with their hosts that started in the past to support holobiont adaptation to the Antarctic Ocean. The wide suite of bacterial cryoprotective proteins found in Antarctic polychaetes may be useful for the development of nature-based biotechnological applications. *Science Advances (2024), 10(25).*

Microbes, planetary health, and the Sustainable Development Goals

Crowther, Thomas W., Rappuoli, Rino, Corinaldesi, Cinzia, Danovaro, Roberto, Donohue, Timothy J., Huisman, Jef et al. *Cell, 187, (19), 5195 – 5216.*

Microorganisms, including bacteria, archaea, viruses, fungi, and protists, are essential to life on Earth and the functioning of the biosphere. Here, we discuss the key roles of microorganisms in achieving the United Nations Sustainable Development Goals (SDGs), highlighting recent and emerging advances in microbial research and technology that can facilitate our transition toward a sustainable future. Given the central role of microorganisms in the biochemical processing of elements, synthesizing new materials, supporting human health, and facilitating life in managed and natural landscapes, microbial research and technologies are directly or indirectly relevant for achieving each of the SDGs. More importantly, the ubiquitous and global role of microbes means that they present new opportunities for synergistically accelerating progress toward multiple sustainability goals. By effectively managing microbial health, we can achieve solutions that address multiple sustainability targets ranging from climate and human health to food and energy production. Emerging international policy frameworks should reflect the vital importance of microorganisms in achieving a sustainable future.

Editorial: Restoration of coastal marine ecosystems

Osinga R, Danovaro R, Debney A and Pogoda B *Frontiers in Marine Science (2024) 11:1485162.*

At the COP 15 summit in Montreal in 2022, the United Nations adopted the Kunming-Montreal Global Biodiversity Framework (GBF; United Nations Environment Programme, 2022), which includes the ambition to protect 30% of the Earth's land, ocean, coastal areas and inland waters by the year 2030. The so called "30 by 30" initiative for conservation management includes measures for active ecosystem restoration of degraded habitats. Hence, a specific target in the GBF is to effectively restore 30% of the degraded ecosystems by the year 2030. Following this ambition, the period between the years 2020 and 2030 has been proclaimed as the UN Decade for Ecosystem Restoration (United Nations Environment Programme, 2021). Ecosystem restoration started in the terrestrial realm, where nowadays, restoration efforts such as reforestation can be implemented at a multi-millions' hectare scale (De Jong et al., 2021). In contrast, restoration of most marine ecosystems is at present executed only at pilot scale (Bayraktarov et al., 2020). Today, the magnitude of successfully implemented marine restoration projects ranges from a few hundred hectares for seagrasses (Van Katwijk et al., 2016) and oyster reef habitats (Bersoza Hernández et al., 2018) to a few hundred square meters for coral reefs (Boström-Einarsson et al., 2020), respectively. Restoration at larger scales to unfold the desired ecological effects is an important target across all degraded marine habitats and is currently being addressed by roadmaps, e.g. for macroalgal (kelp) forests (1 million ha and 4 million ha by 2040; Eger et al., 2023) and by international networks e.g. for biogenic reefs and oyster habitats (Pogoda et al., 2020). The large difference in the spatial scale of intervention between terrestrial and marine ecosystem restoration could limit the possibilities to achieve the targets of the 30 by 30 initiative. In a perspective on restoration of coastal ecosystems that was published at the start of the UN Decade for Ecosystem Restoration, Waltham et al. (2020) identified a series of uncertainties that complicate the planning for large-scale coastal restoration and impede predictions on the outcomes of such restoration measures. Uncertainties included 1) insufficient availability of successful showcases; 2) the scalability of the approaches used for marine restoration; 3) a lack of business cases associated with marine restoration, and 4) unpredictable effects of climate change. In this Research Topic on Restoration of Marine Coastal Ecosystem, we present new insights on the most recent achievements in marine ecosystem restoration four years after the start of the UN Decade for Ecosystem restoration with reference to the four uncertainties mentioned above.

Effects of seagrass (*Cymodocea nodosa*) restoration on nematode biodiversity

Cristina Gambi, Cinzia Corinaldesi, Antonio Dell'Anno, Roberto Danovaro ***Marine Environmental Research (2024), 193, 106301.***

Seagrass meadows are hot spots of biodiversity and play a key role in the provisioning of ecosystem goods and services but are often subjected to a regression due to a combination of multiple anthropogenic and climate-induced impacts. The

ecological restoration of these habitat-forming species is a priority to reverse biodiversity loss and for the recovery of key ecosystem functions. Here we investigated the effects of seagrass (*Cymodocea nodosa*) restoration action on benthic biodiversity recovery assessed by a time-series analysis carried out for one year. We used nematode assemblages, the most widespread metazoan on global sediments, as a proxy of benthic biodiversity and compared the species richness, expected species number (ES51) and composition in donor and in restored seagrasses and in the adjacent unvegetated sediments. One year after the intervention, nematode biodiversity in restored seagrasses was more like that of the donor site than in unvegetated sediments, suggesting a progressive recovery. Overall, the nematode biodiversity of the restored seagrasses resulted in an intermediate level between unvegetated and pristine seagrass meadows, providing evidence that restoration intervention contributed to biodiversity recovery. Pristine and restored seagrass meadows hosted a high number of exclusive species, which resulted in an increase in the overall biodiversity in the investigated location. Our results indicate that the restoration of seagrass meadows has positive effects on benthic biodiversity and contributes to enhance the local biodiversity.

Case Study of Odelouca Tunnel

by Pedro Pinto, Member EUAS

Short Biography

***Education**: Licentiate in Civil Engineer (6 years course,1965-1971) (with honors); from 1971 to 1975 worked with Industry; Master of Engineering (1975 – 1977) (with high honors); 1977-1978 – Fulbright scholarship granted by USA with training periods in MIT (Boston, USA), United States Bureau of Reclamation (Denver), and University of California (Berkeley); Specialist in Geotechnique (Ph.D Level) 1979 - 1983 (with high honors); from 1992 – Director of Research (Full Professor level) (with high honors).*

***ISSMGE** Appointed ISSMGE Board member (2017-2022), and before Immediate Past President (2009-2013), President (2005-2009), Vice President for Europe (2001-2005) and Chairman of TC4 "Earthquake Geotechnical Engineer Committee" (1994-2000).*

***Positions:** President of Scientific Committee of XVII ECSMGE (2024),*

- Member of the European Union Academy of Sciences
- Fellow of the Portuguese Institute of Engineers
- Research Director of LNEC (currently retired)
- Full Professor of Geotechnical Engineering of University of Coimbra (1995-2005, currently retired),
- 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).

***Professional Experience**: 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, Tunisia, Uganda, Venezuela and Zambia, covering field and laboratory testing, dynamic analyses, earthquake engineering, numerical analyses, ground improvement, slopes, special foundations, instrumentation and safety evaluation.*

***Lectures**: He has presented more than 350 State-of-the Art Lectures and Special Lectures in 80 countries of the 5 Continents.*

***Awards**: Pedro Sêco e Pinto has received more than 50 international Awards including 3rd Victor de Mello Lecture, 3rd Braja Das Lecture, 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.*

***Journals**: 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" and SEAG Journal.

- Editor of Proceedings of 6 International Conferences.
***Author/Co-Author**: 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 14 books.*

1. Introduction

Tunnels were hand-dug by several ancient civilizations in the Indian and Mediterranean regions. In addition to digging tools and copper rock saws, fire was sometimes used to heat a rock obstruction before dousing it with water to crack it apart. The cut-and-cover method-digging a deep trench, constructing a roof at an appropriate height within the trench, and covering the trench above the roof (a tunneling technique still employed today)-was used in Babylon 4,000 years ago.

The first advance beyond hand-digging was the use of gunpowder to blast a 515-ft (160-m) long canal tunnel in France in 1681. The next two major advances came about 1850. Nitroglycerine (stabilized in the form of dynamite) replaced the less powerful black powder in tunnel blasting. Steam and compressed air were used to power drills to create holes for the explosive charges. This mechanization eventually replaced the manual process made famous by John Henry, the "steel-driving man," who swung a 10-lb (4.4-kg) sledge hammer with each hand for 12 hours a day, pounding steel chisels as deep as 14 ft (4.2 m) into solid rock.

Between 1820 and 1865, British engineers Marc Brunel and James Greathead developed several models of a tunneling shield that enabled them to construct two tunnels under the Thames River. A rectangular or circular enclosure (the shield) was divided horizontally and vertically into several compartments. A man working in each compartment could remove one plank at a time from the face of the shield, dig ahead a few inches, and replace the plank. When space had been dug away from the entire front surface, the shield was pushed forward, and the digging process was repeated. Workers at the rear of the shield lined the tunnel with bricks or cast iron rings.

In 1873, American tunneler Clinton Haskins kept water from seeping into a railroad tunnel under construction below the Hudson River by filling it with compressed air. The technique is still used today, although it presents several dangers. Workers must spend time in decompression chambers at the end of their shift - a requirement that limits emergency exits from the tunnel. The pressure within the tunnel must be carefully balanced with the surrounding earth and water pressure; an imbalance causes the tunnel either to collapse or burst (which subsequently allows flooding).

Soft soil is prone to collapse and it can clog digging equipment. One way to stabilize the soil is to freeze it by circulating coolant through pipes embedded at intervals throughout the area. This technique has been used in the United States since the early 1900s. Another stabilization and waterproofing technique widely used since the 1970s is to inject grout (liquid bonding agent) into the soil or fractured rock surrounding the tunnel route.

Shotcrete is a liquid concrete that is sprayed on surfaces. Invented in 1907, it has been used as both a preliminary and a final lining for tunnels since the 1920s.

In 1931, the first drilling jumbos were devised to dig tunnels that would divert the Colorado River around the construction site for Hoover Dam. These jumbos consisted of 24-30 pneumatic drills mounted on a frame welded to the bed of a truck. Modern jumbos allow a single operator to control several drills mounted on hydraulically controlled arms.

In 1954, while building diversion tunnels for the construction of a dam in South Dakota, James Robbins invented the tunnel boring machine (TBM), a cylindrical device with digging or cutting heads mounted on a rotating front face that grinds away rock and soil as the machine creeps forward. Modern TBMs are customized for each project by matching

the types and arrangement of the cutting heads to the site geology; also, the diameter of TBM must be equal to the diameter of the designed tunnel (including its lining).

Tunnels have many uses: for mining, for transportation, including road vehicles, trains, subways, and canals and for conducting water and sewage. Underground chambers, often associated with a complex of connecting tunnels and shafts, are increasingly being used for such things as underground hydroelectric-power plants, ore-processing plants, pumping stations, vehicle parking, storage of oil and water, water-treatment plants, warehouses, and light manufacturing; also command centers and other special military needs.

After this brief introduction, the ITA requirements are presented and the case study of Odelouca tunnel is addressed.

2. ITA Requirements

Following the International Tunnelling Association (ITA) the basic documents for tunnel design should include or cover:

The geological report presenting the results of the geological and geophysical survey;

The hydrogeological aspects;

The geotechnical report on site investigations, including the interpretation of the results of site and laboratory tests with respect to the tunnelling process, soil and rock classification, etc.;

Information online, cross-section, drainage, and structural elements affecting later use of the tunnel;

Plans for and a description of the projected excavation or driving procedure, including the different cross-sections related to different ground conditions;

Design documents for the types of excavation methods and tunnel supports likely to be applied, considering, e.g. excavation advance and face support (types and number of anchors, shotcrete strength, closure length, etc.);

The programme for the in-situ monitoring of the tunnel by field measurements;

The analysis of stresses and deformations (for unlined tunnels as well as for single-or double-lined tunnels), and the dimensioning of the tunnel support for intermediate phases and final linings;

The design for waterproofing or drainage;

Structural documents for the final design of the tunnel project, including the detailing;

During and after the excavation, reports on the field measurements and interpretation of their results with respect to the response of the ground and the structural safety of the tunnel;

Documentation of the problems encountered during the excavation and measures applied, e.g. strengthening the ground or changing the projected type of support, based on monitoring results;

Concerning site investigations, the following aspects should be considered for the geological description of each zone:

Name of the geological formation following a genetic classification;

Geologic structure and fracturing of the rock mass with strike and dip orientations;

Colour, texture and mineral composition;

Degree of weathering;

Parameters of the rock mass e.g. in five classes of intervals, including:

Thickness of the layers.

Fracture intercept;

Rock classification;

Core recovery;

Uniaxial compressive strength of the rock, derived from laboratory tests;

Angle of friction of the fractures (derived from laboratory direct shear tests);

Strength of the ground in on-site situations;

Deformation properties (modulus);

Effect of water on the rock quality;

Seismic velocity. Primary stress field of the ground.

3. Case Study of Odelouca tunnel

3.1. Introduction

The site investigation programme is described. For the design of primary lining of Odelouca tunnel Bieniaswki RMR classification and Barton Q system classifications were used. The final tunnel support was designed based in f.e.m analyses.

3.2 Site Investigation

The site investigation has included:

(i) Boreholes with SPT and sampling for laboratory tests;
(ii) Installation of piezometers in some boreholes to measure the water level;
(iii) Geophysical tests, namely crosshole tests and georadar survey,
(iv) Rainfall data;
(v) Pumping tests;
(vi) Laboratory tests, namely identification tests, oedometer tests, uniaxial compression tests.

3.3 Bieniawski's Rock Mass Rating classification (RMR) and recommendations

After analyzing the elements of the geotechnical survey, including boreholes and surface surveys, it is estimated the value of RMR (Rock Mass Rating), Bieniawski (1989) for the 2 geotechnical areas considered.

The RMR Rock Mass Rating system is the most used for rock mass classification (Bieniawski, 1984). It's based on the quantification of six geological and geotechnical parameters and in the attribution of the relative weights. The result of the RMR classification for a specific rock mass can range from 0 to 100, and it's obtained by the algebraic sum of the mentioned parameter weights.

The parameters considered in the classification are:

Strength of intact rock material, with ratings ranging from 0 to 15;

Drill core quality (RQD), 3 to 20;

Spacing of discontinuities, 5 to 20;

Condition of discontinuities, 0 to 30;

Groundwater, 0 to 15;

Adjustment for joint orientation, -12 to 0.

For the types of ground to be crossed the recommendations of the Bieniawski classification are presented in Table 1.

Table 1. Bieniawski classification

Rock mass class	Excavation	Rock bolts (20 mm diameter, fully grouted)	Shotcrete	Steel sets
I - Very good rock *RMR*: 81-100	Full face. 3 m advance.	Generally no support required except spot bolting.		
II - Good rock *RMR*: 61-80	Full face . 1-1.5 m advance. Complete support 20 m from face.	Locally, bolts in crown 3 m long, spaced 2.5 m with occasional wire mesh.	50 mm in crown where required.	None.
III - Fair rock *RMR*: 41-60	Top heading and bench 1.5-3 m advance in top heading. Commence support after each blast. Complete support 10 m from face.	Systematic bolts 4 m long, spaced 1.5 - 2 m in crown and walls with wire mesh in crown.	50-100 mm in crown and 30 mm in sides.	None.
IV - Poor rock *RMR*: 21-40	Top heading and bench 1.0-1.5 m advance in top heading. Install support concurrently with excavation. 10 m from face.	Systematic bolts 4-5 m long, spaced 1-1.5 m in crown and walls with wire mesh.	100-150 mm in crown and 100 mm in sides.	Light to medium ribs spaced 1.5 m where required.
V – Very poor rock *RMR*: < 20	Multiple drifts 0.5-1.5 m advance in top heading. Install support concurrently with excavation. Shotcrete as soon as possible after blasting.	Systematic bolts 5-6 m long, spaced 1-1.5 m in crown and walls with wire mesh. Bolt invert.	150-200 mm in crown, 150 mm in sides, and 50 mm on face.	Medium to heavy ribs spaced 0.75 m with steel lagging and forepoling if required. Close invert.

Primary support recommendations for Bieniawski's 1989 RMR classification. In blue:

for values RMR>70, in green, for values between 50 and 70, in yellow for the interval of RMR 30-50: and finally in red for RMR<30.

3.4 Barton's Q-System Classification and recommendations

The Q system was developed by Barton *et al.* (1974) who, after the observation and analysis of a great number of tunnels in Scandinavia, proposed a quality index Q, for the purpose of rock mass classification and evaluation of primary support requirements. The numerical value of the Q index varies in a logarithmic scale from 0.001 to a maximum of 1000, and is defined by:

$$Q = \frac{RQD}{J_n}\frac{J_r}{J_a}\frac{J_w}{SFR} \quad (1)$$

- RQD/Jn - Represents the structure of the rock mass, crudely measures the compartmentation of the rock mass and its block size.
- Jr/Ja - Represents the roughness and the frictional resistance of the joints.
- Jw/SRF - Represents an empirical factor related with the tensional state of the rock mass designated as "active tension".

In the calculation of the Q value, each parameter can vary ranging between the following values (Barton 1994):

- Rock Quality Designation (RQD), with rating ranging from 0 to 100;
- Joint set number (Jn) 0.5 to 20;
- Joint roughness number (Jr) 0.5 to 4;
- Joint alteration number (Ja) 0.75 to 24;
- Water reduction factor (Jw) 0.05 to 1;
- Stress Reduction Factor (SRF) 2.5 to 10.

Picking the intervals of quality defined for the classification of the rock mass with Bieniawski's RMR classification (boundaries with RMR =30, 50 and 70, converted to Q-System with the expression RMR=15.logQ+50, and entering them in the abacus (Figure 1), (with boundaries at Q=0.05, 1 and 20) it's possible to arrive to primary support requirements and recommendations.

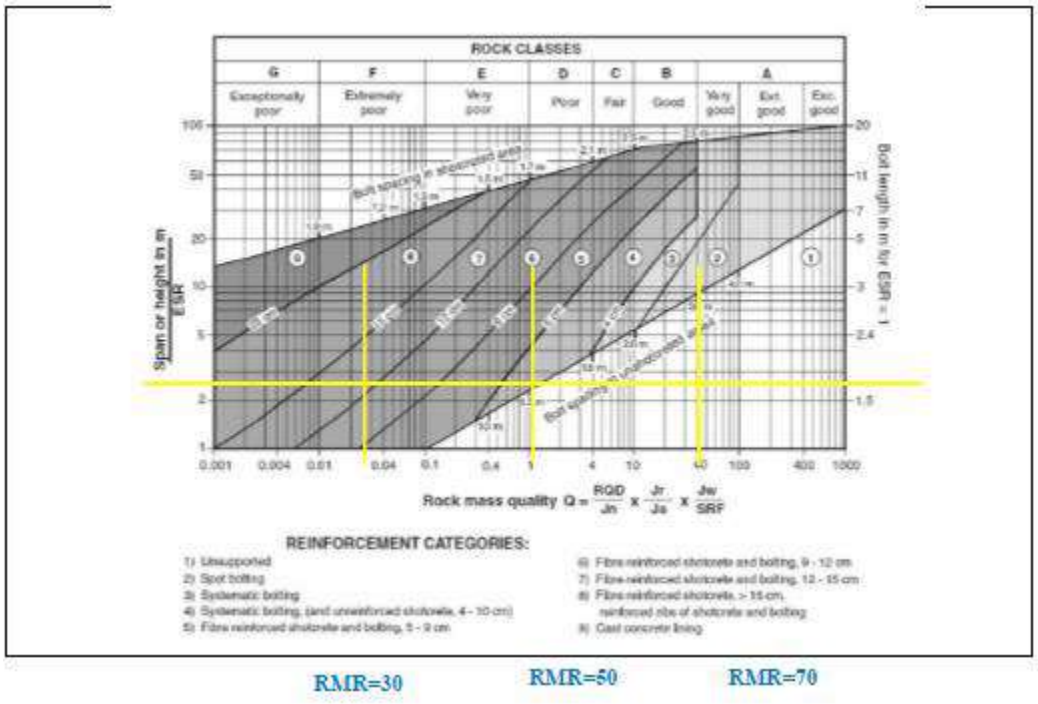

Figure 1. Abacus primary support recommendations

So, the Bieniawski interval values are directly transposed to Q values, using the correlation, another option would be to directly calculate the Q values. For a first approach to primary support and easier comparison of results, only the direct transposition is considered. For entering the abacus, also a ESR - *Excavation Support Ratio* of 1.3 is considered for an excavation around 9.6 m, which results in an equivalent diameter $D_e = 7.4$.

For the massif with **RMR>70**, the tunnels fall in fields 1 and 2 of the abacus, with recommendations of no support requirements and spot bolting.

In the massif quality interval with **RMR 50-70**, the primary support recommendations for fields 3, 4 and 5 range from systematic bolting (spacing of 2.4 m) to 5 to 9 cm of reinforced shotcrete and bolting (spacing of 1.7 m).

At **RMR 30-50** rock mass quality interval, the recommended support requirements range from 9 to 15 cm of shotcrete and rock bolts with spacing between 1.25 and 1.7 m.

For **RMR<30** rock mass quality interval, the tunnel falls inside the fields 8 and 9 of the abacus, and the recommended support requirements range from reinforced shotcrete >15 cm thickness reinforced with ribs and bolting to cast concrete lining.

The recommended rock bolt length, obtained with the expression L=2+(0.15B)/ESR, where B= span, is of 3.1 m.

The maximum unsupported span can be estimated with the expression $2.ESR.Q^{0.4}$. The values obtained, at the boundaries of the geotechnical zones intervals are of 0.78 m for Q=0.05, 2.6 m for Q=1 and 8.61 m for Q=20.

For geotechnical zone 1, with failure of blocks, support of nailing/rock bolts for roof and side walls with 6 m long, 76 mm of diameter and reinforcements of 32 mm, with concrete lining 2, 5 cm thick and metallic mesh was used.

In zone 2 with failure of blocks and slipping a primary lining with concrete of 5 cm thick, and nails 6 m long, 76 mm of diameter and reinforcements of 32 mm (3m apart in

current zones and 1.5 m in more critical zones) was used. Also in some critical zones reinforcement with steel ribs was adopted.

3.5 F.E.M Analysis

A f.e.m. analysis was performed and two situations were analysed: (i) for material ZG1 (material of best quality) a tunnel was analysed with excavation in total section without support, and plastified zones in side walls were identified; (ii) for material ZG2 (material of medium quality) the tunnel was analysed and excavation was simulated in two phases. Plastification in the first phase occurred in the opening and base of the tunnel, but no occurrence of plastification during the second phase.

Due to the occurrence of plastified zones during the opening of the tunnel a primary lining was used. For zone ZG1 gunite 7 cm thick with steel mesh, type Malhasol, was applied.

Also for zone ZG2 application of gunite 7 cm thick with steel mesh, type Malhasol, and the use of nails in the roof was recommended.

Based in f.e.m. analysis the final reinforcement was designed to face the internal and exterior pressure of decompressed rock. For the final support reinforced concrete with 0.30 m thick was used.

3.6 Construction Issues

The application of sprayed concrete is presented in Figure 2.

The use of steel ribs in some critical zones is shown in Figure 3.

3.7 Final comments

The Bieniaswki RMR classification and the Barton Q system classification were useful for the design of the primary lining of Odelouca tunnel.
The f.e.m. analysis was important to identify the plasticity zones and to define the final support.

Figure 2. Application of sprayed concrete in Odelouca tunnel

Figure 3. View of Odelouca tunnel with steel ribs

Figure 4. Odelouca tunnel entrance

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Elasto-Plastic Response of Thick Plates Built in Functionally Graded Material Using the Third Order Plate Theory

by Michał Kleiber, Member EUAS

Short Biography

Prof. Michał Kleiber pursues research in theoretical and applied mechanics as well as information science and applied mathematics. The main subject of his research are applications of state-of-the-art computational techniques in different areas of scientific research, technology and medicine – particularly for modeling, analyzing, simulating and visualizing of complex non-linear thermo-mechanical phenomena.

In recent years, he has been actively involved in research and promotion of national innovation policies.

Biography of prof. MICHAŁ KLEIBER Prof. M. Kleiber was born on 23rd January 1946 in Warsaw. Between 1995 and 2002, Professor Kleiber was the director of the Institute of Fundamental Technological Research of the Polish Academy of Sciences, where since 1986 he has been chairman of the Department of Computational Science and Engineering. In the years 1998-2002 he was member of the Academy's Presidium and between 1997-2001 he chaired the Board for Directors of the Academy's research institutes. In 2007 he was elected the President of the Polish Academy of Sciences and re-elected to this post in 2011. Prof. Michał Kleiber pursues research in theoretical and applied mechanics as well as information science and applied math. The main subject of his research are applications of state-of-the-art computational techniques in different areas of scientific research, technology and medicine – particularly for modeling, analyzing, simulating and visualizing of complex non-linear thermo- mechanics phenomena. In recent years, he has been actively involved in research and promotion of national innovation policies. Professor Kleiber is an author or coauthor of over 280 scientific articles and 7 books published by internationally renowned publishing houses. He is a member of editorial boards of 14 leading international scientific journals and the editor-in-chief of the prestigious Archives of Computational Methods in Engineering (Springer) as well as the journal of Computer Assisted Methods in Engineering Science (IPPT). He has also been active in popularizing science by, among others, being a scientific board member for the popular-science journal Science and Life. Prof. Kleiber is a winner of many awards, including the most prestigious Polish scientific award conferred by the Foundation for Polish Science and the medal granted by the Kingdom of Belgium for innovation achievements. He has been awarded the title of doctor honoris causa by the universities in Lublin, Kraków, Warsaw, Bydgoszcz, Dabrowa Gornicza and Szczecin in Poland, Darmstadt (Germany), Mons (Belgium) and The Polish University Abroad, London, U.K. He also holds the title of ingenieur honoris causa from the Ecole National d'Ingenieurs in Metz (France). He is a foreign member of the Austrian Academy of Sciences, member and former vice-president of the European Academy of Sciences and Arts in Salzburg and member of the Academia Europaea in London. He is a full member of the Warsaw Learned Society. For some 15 years Prof. Kleiber lectured and did research during long-term stays at a number of renowned universities world-wide: in Stuttgart, Hannover, Darmstadt and Bochum in Germany; Berkeley, CA and Stoors, CN, USA; Tokyo, Japan; Hong Kong, among many others. In the years 1998-2001 Michał Kleiber represented Poland in the EU Joint Research Centre as a member of the Board of Governors and in the "Sustainable Growth" Steering Committee in the 5th Framework Programme. Between 2001 and 2005, he headed the Ministry of Science and Information Technology in the Polish government. From 2002 to 2005, Prof. Kleiber was also the chairman of the Governmental Committee for Offset Contracts. In 2005, he was elected member of the European Research Council (Brussels) and chairman of the European Materials Forum (Strasbourg). In the years 2008

– 2010 he was member of the Governing Council Steering Committee of the European Science Foundation in Strasbourg. He also served as the pro bono science and technology advisor to the President of the Republic of Poland (2006 – 2010).
He has received prestigeous national orders and distinctions from the authorities in Poland, France, Belgium, Austria and Greece.

Selection of articles in leading international journal (about 280 together)

Elasto-Plastic Response of Thick Plates Built in Functionally Graded Material Using the Third Order Plate Theory

We present an application of the third-order plate theory for investigation of the elasto-plastic response of thick plates made of functionally graded material.The theory was originally developed by Reddy and Kim [1]. In their formulation they expanded the in-plane displacements up to the cubic term and the transverse displacement up to the quadratic term with respect to the coordinate perpendicular to the plate surface, obtaining a quadratic variation of the transverse shear strains through the plate thickness. FGM properties are modelled following the power law distribution of constituent ratio across the thickness. The plates are modelled using a 16-noded lagrangian elements using Lobatto integration rules. The problem is solved using Newton-Raphson method applying modified Crisfield constant arc-length procedure. Numerical examples are provided to illustrate the advantages of the method proposed.

Buckling and post-buckling analysis of FGM plates resting on the two-parameter Vlasov foundation using general third-order plate theory

We present a nonlinear finite element analysis to investigate the buckling and post-buckling behaviour of functionally graded material (FGM) plates resting on the elastic foundation. The material properties are assumed to vary gradually across the thickness according to a power law distribution. The starting point of the investigation is the generalized third-order plate theory and the Vlasov model of elastic foundation having properties varying throughout the depth. The plates are subjected to bending to verify the formulation and compression loads including buckling and post-buckling analysis to investigate the influence of various parameters on the structural response.

Analysis of FGM plates based on physical neutral surface using general third-order plate theory

We present a nonlinear finite element analysis to investigate the nonlinear behaviour of functionally graded materials (FGM) plates. The material properties are assumed to vary gradually across the thickness according to a power law distribution. The starting point of the investigation is the generalized third-order plate theory which is modified in the present analysis to include the position of the

neutral surface and enhanced with additional terms to represent the distribution stresses better. The plates are subjected to bending and compression loads including buckling and post-buckling analysis.

Gap flow simulation methods in high pressure variable displacement axial piston pumps

A 16-node locking-free Mindlin plate resting on two-parameter elastic foundation - static and eigenvalue analysis

The Pasternak elastic foundation model is employed to study the statics and natural frequencies of thick plates in the framework of the finite element method. A new 16-node Mindlin plate element of the Lagrange family and a 32-node zero-thickness interface element representing the response of the foundation are used in the analysis. The plate element avoids ill-conditioned behaviour due to its small thickness. In the case of the eigenvalue analysis, the equation of motion is derived by applying the Hamilton principle involving the variation of the kinetic and potential energy of the plate and foundation. Regarding the plate, the firstorder shear deformation theory is used. By employing the Lobatto numerical integration in which the integration points coincide with the element nodes, we obtain the diagonal form of the mass matrix of the plate. In practice, diagonal mass matrices are often employed due to their very attractive timeintegration schemes in explicit dynamic methods in which the inversion of the effective stiffness matrix as a linear combination of the damping and mass matrices is required. The numerical results of our analysis are verified using thin element based on the classical Kirchhoff theory and 16-node thick plate elements.

Elastic-plastic buckling and postbuckling finite element analysis of plates using higher-order theory, International Journal of Structural Stability and Dynamics,

Sensitivity analysis of metal forming processes involving frictional contact in steady state

A simple element to model frictional contact in steady state metal forming processes is presented together with the sensitivity analysis to the friction coefficient in a Coulomb friction law. The interest of such model arises from the analysis of rolling processes and a two dimensional approach to cutting problems, where the contact zone is to be determined, however a stationary state is present in most part of the operation. The flow approach proves to be an adequate method to handle efficiently this situation. The contact elements impose a restriction in the velocity component normal to the boundary and a tangential friction force opposite to the velocity. The parts of the boundary which are not in closed contact are treated as free surfaces, which must fulfill the condition of being streamlines. Sensitivity analysis with respect to the friction coefficient is performed by the Direct

Differentiation Method (DDM). The effect of variations in this parameter is discussed for the simulation of an extrusion and a cutting problem.

Incremental finite element sensitivity analysis for nonlinear applications

Finite element formulations for structural sensitivity analysis of non-linear systems with fixed overall shape are discussed. Both the direct differentiation and adjoint variable methods are employed. The resulting sensitivity algorithms are consistent with time integration scheme adopted for solving equilibrium problem. Effectiveness and computational aspects of the procedures are discussed and compared. Numerical algorithms are shown to be readily implemented in existing finite element codes. Large-scale examples illustrate the paper.

Modeling and numerical-analysis of stresses and strains in the human lung including tissue-gas interaction

A complete mechanical model of lungs, valid for the analysis of stresses in tissues, which considers mechanical couplings between the tissue deformation and the air flow, is presented. The concept of a continuous description of the lung is adopted, with its volume assumed to be filled with a nonlinearly elastic, highly deformable solid - parenchyma, which is a thin-walled porous tissue structure on the micro-scale. Central airways are modelled as a discrete system of conduits immersed in the parenchyma. For the flow in peripheral airways and alveoli, a model of filtration in a three-dimensional two-phase porous medium (gas-tissue skeleton) is assumed. A new approach to pseudoelastic nonlinear constitutive modelling of parenchyma aiming at computational applications is presented. A fundamental set of nonlinear differential equations for the quasi-static coupled problem is derived and frictionless contact boundary conditions are included. A finite element formulation of the problem with an implicit time integration scheme is presented. The results of numerical examples obtained using the algorithm agree qualitatively with experimental data.

Numerical limit analysis of perforated plates

Full limit analysis is presented of a thin plate under plane stress, perforated with circular holes arranged in a regular penetration pattern. The material is assumed to be elastic–perfectly plastic and to obey the Huber–Mises yield condition together with its associated flow law. The finite element tangential stiffness method is employed. Triangular constant-strain elements are used, the load being generated by means of constant edge displacements at the periphery of a suitably selected subregion. Load-displacement diagrams are obtained for various edge displacement programs and then an interaction curve is constructed for the perforated plate considered. Each computational step is associated with a certain plastic zone which develops until the limit state configuration is reached. The plate is provided with equilateral triangular configuration of holes with arbitrary cutout coefficients. The

interaction curves are plotted against the Huber–Mises yield condition for the plate without openings.

Selection of books

The stochastic finire elemnt method, Wiley
Incremental finite element modeling in non-linear solid mechanics, Ellis Horwood
Introduction to nonlinear thermomechanics of solids, Springer
Finite element mthods in structiural mechanics, Ellis Horwood
Nonlinear structural mechanics. Kluwer Academic Publishers
Artificial Intelligence in computational engineering, Ellis Horwood

A Novel Beam Element with Nine DOFs per Node for Resolving the Warping-Distortion Compatibility in Analysis of Frames and Curved Beams made of I-sections

by Yeong-Bin Yang, Member EUAS

Short Biography

Dr. Yeong-Bin Yang received his Ph.D. degree from Cornell University in 1984. He is a member of Chinese Academy of Engineering, EU Academy of Sciences, European Academy of Sciences and Arts, and foreign member of Austrian Academy of Sciences. Currently, he is Honorary Dean of Civil Engineering, Chongqing University, 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 President of National Yunlin University of Science and Technology (Yuntech), Dean of NTU College of Engineering, Chairman of NTU Civil Engineering Department, and President of four societies in Taiwan: Institute of Engineering Education Taiwan (IEET), Chinese Institute of Civil and Hydraulic Engineering (CICHE), Society of Theoretical and Applied Mechanics (TAM), and Chinese Society of Structural Engineering (CSSE). He has published over 300 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. He has a Google citation of 16,670 times and H index of 65. Recently, he received the Zienkiewicz Medal from APACM and the Lifetime Achievement Medal from ASCE Greater China Section.

Below are the abstracts of three papers that have been published in 2024:

1. Thin-walled Structures 194 (2024) 111314

A novel beam element with nine DOFs per node for resolving the warping-distortion compatibility in analysis of frames and curved beams made of I-sections

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Abstract: Warping-distortion coupling is common in frames and curved beams made of I-sections, which tends to decrease significantly the lateral and torsional resistance of structures. Traditionally, it has been difficult to consider such effects in structural analysis, because the warping and distortional degrees of freedom (DOFs) of two connected elements at a common joint cannot be easily transformed to a common coordinate system for global stiffness assembly. The purpose of this paper is to conquer such a problem. By introducing the symmetric and anti-symmetric distortion modes, in addition to the warping and conventional six DOFs, this paper develops a new theory that consists of nine DOFs per node for the two-node I-beam element. The three deformational DOFs of the cross-section, i.e., the symmetric distortion, anti-symmetric distortion and warping, can be regarded as three mechanical couples relating to the twisting, shearing and bending, respectively, of the two flanges in the opposite sense. This allows all the DOFs of the connected elements at a common joint to be easily transformed to the global coordinates for stiffness assembly. As a result, the warping-distortion compatibility problem that occurs in frames and curved beams is resolved. In the exemplar studies, the present beam element has been demonstrated to be capable of producing results that are in excellent agreement with those of the shell element for the lateral deformation of angled frames with unstiffened and stiffened joints and of curved beams with various boundary conditions. It is also observed that the cross-sectional distortion effect becomes more manifest in curved I-beams of high curvature or of high flange-to-web rigidity ratio.

Keywords: Cross-sectional distortion, curved beam, frame, I-beam, thin-walled beam, warping.

2. International Journal of Structural Stability and Dynamics
Vol. 24, No. 15 (2024) 2471006

Bridge damping formula based on correlation between the front and rear contact responses of a two-axle scanning vehicle

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Abstract: In this note, a simple formula is derived for the modal damping ratio of the bridge using the correlation between the instantaneous amplitudes of the related front and rear contact responses of a two-axle test vehicle by the Hilbert transform (HT). To start, closed-form solutions were derived for the dynamic response of the damped bridge and vehicle-bridge contact responses. Next, the HT was employed to generate the instantaneous amplitudes of the two contact points. Based on their correlation, a simple formulate is derived for the bridge damping ratio. Finally, the reliability of the derived formula was verified in the numerical study. It was demonstrated that the proposed formula can be successfully used to determine the bridge damping ratio, even in the presence of rough pavement, but with the aid of random traffic.

Keywords: Bridge; vehicle scanning method; contact; damping ratio; Hilbert transform.

3. Mechanical Systems and Signal Processing 208 (2024) 111026

Novel formula for determining bridge damping ratio from two wheels of a scanning vehicle by wavelet transform

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Abstract: A novel formula is derived for determining the bridge damping ratio from the correlation of the front and rear wheels of a test vehicle using the modal components extracted by the wavelet transform (WT). Firstly, closed-form solutions are derived for the dynamic responses of the bridge under a moving two-axle vehicle. Next, to remove the masking effect by

vehicle's frequencies, the wheel-bridge contact responses back-calculated from the vehicle responses are used in analysis. Then, the WT is employed to obtain the instantaneous amplitudes of the component responses of the two contact points. Finally, using the correlation between the two contact points, a novel formula is derived for the bridge damping ratio. The above derivations are validated by numerical simulations. Through the theoretical analysis and numerical simulations, the following conclusions are made: (1) the spatial correlation of the front and rear contact points is utilized to derive the bridge damping formula using the WT; (2) for multi-span bridges, the RANdom SAmple Consensus (RANSAC) can beneficially downplay the data points with large deviations near the internal supports in fitting the bridge damping ratio; (3) the first span can be reliably used to calculate the damping ratio of multi-span bridges, especially in the presence of pavement roughness; and (4) the formula has been attested to be robust against various levels of vehicle and bridge damping.

Keywords: Bridge; vehicle scanning method; damping ratio; contact; wavelet transform.

Research on Pathogenesis and Chemoprevention of Cancer

by Zigang Dong, Member EUAS

Short Biography

Position:*Professor, Vice President of Zhengzhou University and Dean of Medical College*

Education

1978 – 1983 *M.D., Department of Medicine, Henan Medical University, P.R. China*

1983 – 1986 *M.S., Department of Pathophysiology, Henan Medical University, P.R. China*

1987 – 1991 *Dr. P.H., Mailman School of Public Health, Columbia University, New York*

Positions and Honors

1991 – 1995 *Postdoctoral Fellow, PRI/DynCorp, NCI-Frederick Cancer Research & Development Center, Frederick, MD*

1992 – 1995 *Group Leader, PRI/DynCorp, NCI-Frederick Cancer Research & Development Center, Frederick, MD*

1995 – 1997 *Assistant Professor, The Hormel Institute, University of Minnesota, Austin, MN*

1998 – 1999 *Associate Professor, The Hormel Institute, University of Minnesota, Austin, MN*

1997 – 2019 *Full Member, Cancer Center, University of Minnesota, Minneapolis, MN*

2001 – 2019 *Executive Director, The Hormel Institute, University of Minnesota, Austin, MN*

2000 – 2019 *Full Professor, The Hormel Institute, University of Minnesota, Austin, MN*

2009 – present *Professor with tenure, Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota*

2019 – present *Dean of College of Medicine, Zhengzhou University, Zhengzhou, Henan, China*

2020 – present *Vice president, Zhengzhou University, Zhengzhou, Henan, China*

Awards, Honors and Other Special Scientific Recognition

1999 *The Gallo Award, The Cancer Institute of New Jersey*

2000 *Alice Hamilton Award, Biological Science category, National Institute for Occupational Safety and Health, Centers for Disease Control and Prevention (CDC) for research presented in JBC 274: 30611-30616, 1999 (Publication # HI 1442)*

2001 – 2019 *Hormel/Knowlton Professor, The Hormel Institute, University of Minnesota*

2006 – 2019 *University of Minnesota McKnight Presidential Professor in Cancer Prevention*

2008 – 2014 *National Institutes of Health Merit Award*

2010 – 2019 *Internal Advisory Committee, Center for Translational Science Activities, Mayo Clinic*

2010 *World Class Professor, Seoul National University, South Korea*

2011 – 2015 *External Steering Panel for the Division of Cancer Prevention, NCI, NIH*

2011 *Oh Dang Award, The Pharmaceutical Society of Korea, South Korea*

2012 *Stars in Nutrition and Cancer Lecturer Award, Division of Cancer Prevention, NCI, NIH*

2013 – 2019 *I.J. Holton Professor, The Hormel Institute, University of Minnesota*

2013 *International Science and Technology Collaboration Award, Hunan, China*

2014 *Yellow River Friendship Award, China*

2016 *Outstanding Achievement Award, Society of American Asian Scientists in Cancer Research*

2020 *The 8th Overseas Chinese Contribution Award, China*

2020 *Science and Technology Collaboration Award, Henan, China*

2023	*Foreign Full Member, Academician of the Russian Academy of Engineering*

Editorial Work

2004 – 2008	*Carcinogenesis: Editorial Board member*
2003 – 2010	*Journal of Biochemistry and Molecular Biology: Overseas Editor*
2005 – present	*Molecular Carcinogenesis: Associate Editor*
2003 – present	*Biofactors: Editorial Board member*
2006 – present	*International Journal of Biological Sciences: Editorial Board member*
2007 – 2013	*Cancer Research: Editor*
2008 – 2015	*Cancer Prevention Research: Editorial Board member*
2015 – present	*Cancer Prevention Research: Senior Editor*
2010 – 2014	*Carcinogenesis: Editorial Board member*
2011 – 2019	*The Journal of Biological Chemistry, Editorial Board member*
2014 - 2019	*EBioMedicine Editorial Board member*
2016 – 2019	*Nature Partner Journal: Precision Oncology: Editor-in-Chief*

Professor Zigang Dong has long been engaged in research on the pathogenesis and chemoprevention of cancer, and has original achievements with international influence in the field of carcinogenic mechanisms and chemoprevention of physical and chemical carcinogens. He is a leader in cancer chemoprevention research in the world. Professor Dong has published over 580 articles in journals such as Nature, Nature Reviews Cancer, Nature Cell Biology, Nature Structure and Molecular Biology, and Science Signaling, with a total citation of over 41000 times. Serving as an editorial board member or deputy editor in chief of various authoritative journals in the field of cancer research, such as Cancer Research、Cancer Prevention Research and Carcinogenesis. Professor Dong has signed a contract with Nature Publishing Group to establish the magazine 'npj Precision Oncology'. He has received the highest honor of McKnight Chair Professor at the University of Minnesota. Professor Dong won Gallo Award in 1999 and the Merit Award from the National Institutes of Health in 2008. In 2012, he received the Nutrition and Cancer Star Award from the American Cancer Institute. In 2013, he was awarded the I. J. Holton Chair Professor at the University of Minnesota. In 2014, Professor Dong won the Yellow River Friendship Award from the Henan Provincial Government. In 2016, he was awarded the Outstanding Contribution Award by the Asian American Cancer Society. In 2020, he won the 8th China Overseas Chinese Contribution Award and the Henan Province Science and Technology Cooperation Award. In 2021, he was selected as the "Top 100000 Scientists in the World", ranking the third in clinical medicine in Chinese Mainland and the first in all scientific fields in Henan Province. In the same year, he was selected as professor in national level. In 2023, elected as a foreign academician of the Russian Academy of Engineering. In 2024, elected as a member of the European Academy of Sciences. In the same year, he was invited to attend the National Day reception celebrating the 75th anniversary of the founding of the People's

Republic of China. Professor Dong has been selected multiple times for the "Top 2% Global Scientists List", and in 2024, he was selected for the "career-long impact Scientists", ranking first in all scientific fields in Henan Province.

Professor Dong is a world leader in cancer prevention and molecular carcinogenesis. He conducted pioneering work in elucidating physical and chemical carcinogen-induced signal transduction pathways as molecular targets for chemopreventive agents in carcinogenesis. He has systematically and innovatively studied the molecular targets and mechanisms of cancer chemopreventive drugs and established the models or crystal structures for the binding of drugs to their target molecules, which drove the design and clinical trials of new cancer preventive drugs through theoretical breakthroughs. Professor Dong's research group has multiple drugs undergoing phase 0 to IV clinical trials. The National Cancer Institute of the United States highly praises Professor Dong's research work on its website, believing that Professor Dong has pioneered the application of high-tech in the study of carcinogenic mechanisms, cancer treatment target molecules, and cancer prevention drugs. In 2009, Professor Dong was invited to publish a paper titled "Cancer Prevention Research - Then and Now" in Nature Reviews Cancer, systematically elaborating on the progress and research focus of cancer chemoprevention, and becoming a key recommended article on the Nature website.

Professor Dong's group was the first to identify protein kinases including p38, ERKs, JNKs, Fyn, MLTK and RSK as p53 protein kinases that phosphorylate p53 at different amino acid residues. p53, known as the "molecular police," is the most well-known tumor suppressor to date. Professor Dong conducted the first study on the phosphorylation modification of different sites of p53 and its role in cell cycle, apoptosis, and carcinogenesis, and discovered 18 different upstream protein kinases that modify p53 phosphorylation. Invited to publish a review article titled "Post translational modification of p53 in tumor genesis" in Nature Reviews Cancer, it is one of the most cited papers in the field of molecular biology and genetics worldwide from 2003 to 2009 by Thomson Reuters Science Watch.

For the limitation that a single cause cannot explain the occurrence of cancer, Professor Dong proposed a new theory of "1+X" that the main carcinogenic cause combined with multiple carcinogenic factors leads to the occurrence of cancer. He pointed out that the injury of esophageal epithelium caused by hot food and hot drink may be the main reason for the occurrence of esophageal cancer. The prevention strategy based on this theory has been popularized and applied in the high incidence areas of esophageal cancer. In recent years, the incidence rate of esophageal cancer has declined year by year. This theory was published in the authoritative journal of Cancer Research of the American Cancer Society, and is expected to become a global

guideline for cancer prevention. In addition, Professor Dong's team used spatial transcriptomics analysis to sequence specific areas of esophageal squamous epithelial precancerous lesions, and found that the stage of esophageal squamous precancerous lesions was in an immunosuppressive state. The use of machine learning methods to screen and study confirmed that the expression of TAGLN2 significantly increases during the progression of esophageal cancer, while the expression level of CRNN decreases. Further research confirms that TAGLN2 promotes the progression of esophageal cancer, while CRNN inhibits the progression of esophageal cancer. This study suggests that early intervention should be carried out in high-risk populations with abnormal expression of TAGLN2 and CRNN in esophageal precancerous lesions. The research results were published in Nature Communications and were named one of the top 50 papers of 2023 by the journal.

For a long time, H. pylori infection has been considered as the main cause of gastric cancer. However, so far, there is not enough experimental evidence to support this argument. Professor Dong proposed a new theory of "emotional illness" in the occurrence of gastric cancer: Helicobacter pylori infection alone is not enough to cause the occurrence of gastric cancer, the biological factors of Helicobacter pylori infection, chronic stress, alcohol consumption, and other factors work together to lead to the occurrence of gastric cancer. The proposal of this academic idea has attracted widespread attention in the academic community since its publication, and is expected to provide new theoretical basis for exploring the etiology and molecular mechanisms of gastric cancer. In addition, Professor Dong’s research group found that CDK12 is a driver gene in human gastric cancer growth. Mechanistically, CDK12 directly binds to and phosphorylates PAK2 at T134/T169 to activate MAPK signaling pathway. They further identified FDA approved clinical drug procaterol can serve as an effective CDK12 inhibitor, leading to dramatic restriction of cancer cell proliferation and tumor growth in human gastric cancer cells and PDXs. These data highlight the potential of CDK12/PAK2 as therapeutic targets for patients with gastric cancer, and propose procaterol treatment as a novel therapeutic strategy for human gastric cancer, which is of great significance and value for the prevention and treatment of gastric cancer.

Thermal Management of Aerospace Systems

by Tom I-P. Shih, Member EUAS

Short Biography

DR. TOM I-P. SHIH is professor of aeronautics and astronautics at Purdue University, where he served as the head of the School of Aeronautics and Astronautics from 2009 to 2019. Prior to joining Purdue, he was a mechanical engineer at NASA Lewis (now Glenn) Research Center and served on the faculties of the Univ. of Florida, Carnegie Mellon Univ., Michigan State Univ., and Iowa State Univ. (chair of the Dept. of Aerospace Engineering, 2003–2009). Currently, he is the editor-in-chief of the AIAA Journal and serves on the advisory boards of the Dept. of Mechanical Engineering at The Univ. of Michigan and Michigan State Univ. and the Dept. of Mechanical, Materials, and Aerospace Engineering at Illinois Institute of Technology and West Virginia Univ. He also serves on the review board of the Air Force Research Laboratory's Collaborative Center for Aeronautical Sciences. Previously, he has served on the Aeronautics Committee of the NASA Advisory Council (2018-21) and chaired the AIAA Committee on Higher Education (2016-23) and the Aerospace Department Chair Association (2005-06). Dr. Shih started his undergraduate education at West Virginia Univ., but completed his B.S. at the National Cheng Kung Univ. in Taiwan. His M.S.E. and Ph.D. degrees are from The Univ. of Michigan at Ann Arbor. He is a Fellow of the American Institute of Aeronautics and Astronautics (AIAA) and the American Society of Mechanical Engineers (ASME) and received the 2010 Distinguished Engineering Educator Award from the Engineers' Council of San Fernando Valley, the 2015 AIAA Energy Systems Award, the 2020 AIAA Thermophysics Award, Mechanical Engineering Alumni Merit Award from The University of Michigan in 2023, and the NCKU Distinguished Alumni Award from National Cheng Kung University in 2023.

Research Interests

Dr. Shih's research interests are in fluid mechanics, heat transfer, and numerical methods and their application to problems in aerodynamics (airfoils and wings with ice accretion, shock-wave/boundary-layer interactions with bleed, and mixed-compression inlets); energy, power, and propulsion systems (gas turbines, piston and rotary engines, automotive torque converters, automotive clutches, liquid-ring vacuum pumps, thermoelectric power generators); and two-phase flows (electrodeposition; particle/particle and particle/fluid interactions). Current research is on the development of generalizable reduced-order models for the design of turbine cooling that satisfy physical constraints and embed higher dimensional effects; automatic grid generators that embed human intelligence (HI); and thermal management of gas turbine and rotation detonation engines.

Aerospace vehicles and their components are complicated systems that operate in harsh environments with extreme temperatures, pressures, heat

loads, and forces. Examples include hypersonic vehicles, high-power density electronics, directed energy, thrust vectoring, and gas turbines. For many of these systems, managing the temperature, referred to as thermal management, is paramount for reliability, safety, performance, efficiency, and service life. In the following, selected research by the author connected to the thermal management of gas turbines are briefly outlined.

On gas turbines, thermal efficiency increases with the temperature of the gas entering the turbine component. Those temperatures in advanced gas turbines, up to 2000 ^{o}C for aircraft, far exceed the temperature at which the best material available could maintain structural integrity with minimal creep and thermal fatigue. Thus, cooling is needed for all parts of the turbine material that contact the hot gases. Currently, up to 20% of the air entering the gas turbine's high-pressure compressor is extracted to cool the turbine. Since cooling requires work and the cooling air extracted could be used to produce work, the amount of cooling air extracted must be minimized or the cooling be made more efficient to enable even higher turbine inlet temperatures.

What are the challenges in advancing turbine cooling? There are four, and they are the need for (1) accurate and efficient computational tools for design and analysis, (2) diagnostic tools that could measure the details of the flow and heat transfer in harsh environments, (3) understanding how design and operating parameters affect fluid mechanics and heat transfer, and (4) high-temperature resistant materials and their fabrication with internal and film cooling. Our research has focused on challenges 1, 2 and 3. On these challenges, a special section in the *Journal of Propulsion and Power*[1] and two books in AIAA's *Progress in Astronautics and Aeronautics*[2, 3] have been edited with reviews written by leading researchers to summarize the state of the art.

On computational tools, our research group has developed several models. The first is a Biot-number analogy for design of experiments so measurements made under benign laboratory conditions (e.g., near room temperature and ambient pressure instead of 2000 ^{o}C and 30 bars) could be scaled to provide meaningful normalized temperature distributions in the turbine material as if operating under the harsh conditions.[4] It involves a generalized Biot number that is unique and a function of position for any three-dimensional structure heated on one side and cooled on the other side and a study that showed if it is the temperature distribution in the material that is of interest, then scaling from benign to harsh operating conditions requires this generalized Biot number distribution to be matched. The second is a reduced-order model to estimate the over temperature in the turbine material (i.e., the temperature beyond the maximum permitted for structural integrity) during transient operations and how to prevent over temperature by pre-

cooling.[5] In gas turbines, insufficient cooling that results in just 25 ^{o}C over temperature at any location in the turbine material could reduce the turbine's service life by a factor of two.[6] The third is a reduced-order model to estimate the maximum and minimum local temperatures and their gradients in turbine materials to enhance the capabilities of existing preliminary design tools to account for local variations in heat transfer in internal cooling ducts with heat-transfer enhancement features such as ribs and pin fins without the need to resolve those features.[7] This is important because the heat-transfer coefficient (HTC) between a pair of ribs or pin fins could vary by a factor of eight or more, but existing preliminary design tools use average HTCs that do not account for those variations and so could significantly under predict cooling needs in critical areas and over predict them elsewhere. The fourth is the development of a hybrid large-eddy simulation (LES) method that removes the "gray areas" where regions modelled by LES transitions to regions modelled by the Reynolds-Averaged Navier-Stokes (RANS) equations.[8,9] In addition, a method was developed to extract information from the upstream LES solution to convert a downstream RANS model with a scalar eddy viscosity into a tensorial eddy viscosity that can adaptively reproduce the turbulence structures in the upstream LES region. The fifth is showing why RANS models could not reproduce LES results. Often, the reason is RANS's inability to predict unsteady flow separation, and our research proposed a method so that it could.[10]

On experimental methods, our research has focused on the accuracy of measurement methods for the heat-transfer coefficient and the reference temperature in Newton's law of cooling for internal and film cooling.[11] Humble, et al.[12] showed that for internal cooling (i.e., flow through ducts), if the bulk temperature is used – albeit hard to define for ducts with ribs, pin fins, curvature, and flow separation – then the Nusselt number as a function of Reynolds and Prandtl numbers along with the ratio of the local wall to bulk temperature behaves like an equation of state. However, many experimental studies approximate the bulk temperature, and our research showed that those approximations could create errors up to 30% in the reported heat-transfer coefficient.[13] Also, there are two ways to measure the heat-transfer coefficient and the bulk temperature – steady-state methods and transient methods. Since conduction heat transfer in solids has time scales much longer than those in the gas phase, steady-state methods are time consuming. As a result, many experimental studies use transient methods, which are fast and efficient. On transient methods, our study showed techniques that use the exact solution of the semi-infinite solid could produce substantial errors because the change in the thermal boundary layer with time could significantly change the local bulk temperature and the resulting heat-transfer coefficient about ribs and pin fins.[14] Thus, transient method are not

recommended unless experimentalists can show that the measurements made do not change with time as the thermal-boundary layer changes. For film cooling, the challenge is the reference temperature. Currently, the adiabatic-wall temperature is used, which is the temperature measured or computed on an adiabatic wall. Thus, the adiabatic-wall temperature assumes the reference temperature to be independent of the wall temperature and the wall heat flux. Experimental methods mimic the adiabatic-wall temperature by using solids with very low thermal conductivity (adiabatic-wall BC method) or by using two measurements and then linearly extrapolating (linear-extrapolation method). For the adiabatic-wall BC method, our study showed when the wall temperature equals the adiabatic-wall temperature, the heat flux there is not zero so the heat-transfer coefficient approach plus or minus infinity at locations on the film-cooled surface where the direction of heat flux flips.[15] For the linear extrapolation method, our study showed the adiabatic-wall temperature obtained to be non-unique and could be nonphysical.[15] To overcome these challenges, a thermal mapping method was developed that accounts for upstream heat transfer to ensure that wherever the wall temperature equals the adiabatic-wall temperature, the heat flux there is zero and that the heat-transfer coefficient is continuous there.[15]

On understanding the flow and heat transfer in turbine cooling, studies were made by using RANS, hydrid LES, and LES. Our research group was among the first to use a low-Reynolds number RANS model that also accounted for the effects of compressibility due to the huge temperature differences between the wall and the cooling air – albeit the Mach number is much less than 0.3 – to study internal cooling in straight and rotating ducts with and without ribs.[16-18] The focus was on understanding how secondary flows induced by the Coriolis force from rotation, streamline curvature about curved ducts, and heat-transfer enhancement features such as inclined ribs affect heat transfer under laboratory and engine-relevant conditions. In those studies, centrifugal buoyancy was found to induce flow separation on the leading face of internal cooling duct, which significantly reduce the heat transfer there. On internal cooling, studies were also made to examine effects of dimples and pin fins in straight and tapered ducts with and without rotation[19-24] and effects of wall to bulk temperature ratios (T_w/T_b) from benign laboratory to harsh enngine operating conditions.[25] The study on the effects of T_w/T_b showed designs based on laboratory conditions, where T_w/T_b is near unity, to have significantly over predicted the heat-transfer capabilities of pin fins in the first few rows of pin-fin arrays. On film cooling, our research focused on understanding flow physics[26-29] and on ways to enhance adiabatic effectiveness, which included flow aligned blockers,[30] upstream ramp,[31] W-shaped holes,[32] and downstream vortex generators.[33,34] Our research has also focused of endwall contouring[35] and blade contouring[36] to minimize

horseshoe and passage vortices in the hot-gas path between vanes in the first-stage turbine as well as ingress and egress from rim seals[37,38] that affect aerodynamics and heat loads on vanes and blades.

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Tip Gap Effects on Film Cooling Performance of a Transonic Turbine Blade with a Distinctive Coolant Supply Arrangement

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 2024, Dr. Ligrani is author or co-author of more than 231 publications in archival journals, including the International Journal of Heat and Mass Transfer, the ASME Transactions-Journal of Turbomachinery, the ASME Transactions-Journal of Engineering for Gas Turbines and Power, the ASME Transactions-Journal of Heat Transfer, the ASME Transactions-Journal of Fluids Engineering, the International Journal of Thermal Sciences, 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, Measurement Science and Technology, Applied Thermal Engineering, and the Journal of Microcolumn Separations. He is also author of 11 book chapters, and about 167 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 2023, he has also presented approximately 207 lectures at different institutions and establishments, including many invited lectures. From 2006 to 2023, he presented or is scheduled to present approximately 8 Invited Keynote Papers, 12 Invited Papers, and 12 Invited Plenary Papers at different international conferences. Current SCOPUS Reference Citation H-INDEX is 51. Current GOOGLE SCHOLAR Reference Citation H-INDEX is 57.

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 for the ASME Transactions-Journal of Fluids Engineering from 2005 to 2008. He also served as Associate Editor, ASME Transactions-Journal of Journal of Engineering for Gas Turbines and Power from 2018 to 2021 and from 2021 to 2024.

RESEARCH FUNDING AWARDS

Dr. Ligrani has a strong past and present record of performing sponsored, fundamental and applied research for a variety of funding agencies, including ones in the USA and Europe. As such, he has successfully managed a wide variety of research programs, for different industrial, foundation, and government sponsors. As of December 2024, research funding awards have been received from the following organizations: U.S. Air Force Research Laboratory - Aerospace Systems Directorate, CFDRC – Computational Fluid Dynamics Research Corporation, NASA – Marshall Space Flight Center (MSFC),

Alabama State Innovation Program Fund, University of Alabama in Huntsville Endowment for Eminent Scholar in Propulsion, University of Alabama in Huntsville Start-Up Funds, AEDC – Arnold Engineering Development Center of Arnold Air Force Base, National Science Foundation, Honeywell Aerospace Corp., The Boeing Company, IHI Corporation, the Henry Luce Foundation, South Carolina Institute for Energy Studies (SCIES-AGTSR) of the Department of Energy, U. S. Army Aviation Research and Technology Activity-AVSCOM, NASA-Ames Research Center, NASA-Lewis Research Center, Hispanic Research Center-Arizona State University, Turbo and Power Machinery Research Center-Seoul National University, Solar Turbines Incorporated, UCON U.S.-Japan Center-Weber State University, General Electric Corporate Research and Development Center, Pratt & Whitney Corporation-Florida, the North Atlantic Treaty Organization (NATO), Pratt & Whitney Corporation-Canada Corp., the Gas Technology Institute, Intel Corporation, HEET-High Efficiency Engines and Turbines Program - South Carolina Energy Research and Development Center, Invesys Corp. - Foxboro Company, Ceramatec Advanced Materials and Electrochemical Technologies Corp., CISCO Systems Inc., SEEDA-South East England Development Agency, EPSRC – Engineering and Physical Sciences Research Council of Great Britain, ISIS Innovation, John Fell Fund, European Community Sixth Framework Programme, Korea Institute of Geoscience and Mineral Resources - KIGAM, Lockheed Martin UK, The Royal Academy of Engineering, Rolls Royce PLC, Science and Engineering Research Council (SERC) Engineering Board of Great Britain, Office of Naval Research, Naval Postgraduate School Research Foundation, Aero-Propulsion Laboratory-Wright-Patterson Air Force Base, and Naval Postgraduate School Direct ***Funding.***

CURRENT AND RECENT RESEARCH FUNDING AWARDS

As of December 2024, current and recent research sponsors at the University of Alabama in Huntsville include: (1) Solar Turbines, Inc. of San Diego, California, USA (multiple research contracts), (2) IHI Corp. (Ishikawajma Harima Heavy Industries), of Tokyo, Japan (multiple research contracts), (3) National Science Foundation, CBET Thermal Transport Processes, Division of Chemical, Bioengineering, Environmental, and Transport (CBET) Systems, Arlington, Virginia, USA (multiple funding awards), (4) the Alabama Innovation Fund, Research Program, Montgomery, Alabama, USA, (5) Office of the Vice President for Research and Economic Development, University of Alabama in Huntsville, Huntsville, Alabama, USA, (6) AEDC – Arnold Engineering Development Center, Arnold Air Force Base, Tullahoma, Tennessee, USA (high pressure tank donation), (7) U.S. Air Force Research Laboratory, SBIR/STTR Program, Aerospace Systems Directorate, Wright-Patterson Air Force Base, Ohio, USA, (8) NASA – Marshall Space Flight Center (MSFC), Huntsville, Alabama, USA.

RESEARCH AREAS AND EXPERTISE

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.

TIP GAP EFFECTS ON FILM COOLING PERFORMANCE OF A TRANSONIC TURBINE BLADE WITH A DISTINCTIVE COOLANT SUPPLY ARRANGEMENT.

Considered are the influences of tip gap on film cooling performance variations near to and along the tip or end of a turbine blade with a squealer rim contained within a linear cascade with five airfoils. The film coolant is supplied by two plenums which are positioned at forward and aft locations within the blade. The aft blowing ratio varies between 0.88 and 1.48, the forward blowing ratio is set to be approximately constant in the vicinity of 2.75 to 3.0, and a value of about 1.3 is utilized for the ratio of coolant density relative to the main flow density. Measured results include linearly-averaged and spatially-resolved variations of adiabatic effectiveness, which are presented both for the top portion of the pressure surface and end surface of the blade with the squealer rim. Local effectiveness variations along the top pressure side of the blade show significant effectiveness values downstream of aft pressure side hole outlet locations mostly because film lift-off downstream of these holes is less substantial than observed downstream of the forward holes. Spatially-resolved effectiveness data for the end of the blade with a squealer rim show that the largest values of effectiveness are evident near to and immediately downstream of dusting hole outlet locations. Associated linearly-averaged effectiveness data for the tip of the blade recess region with the 1.2 mm tip gap are as much as about two times higher than values for the 2.0 mm tip gap when compared at each surface location. Local and linearly-averaged surface effectiveness variations for the downstream edge region of the blade squealer tip are most strongly influenced by the film cooling holes which are aft and by the dusting hole which is positioned along the tip of the blade rim near the downstream edge. Here, effectiveness magnitudes are also often higher along the downstream edge rim region with the 1.2 mm tip gap, compared to data associated with the 2.0 mm tip gap.

UNSTEADY RELATIONSHIPS BETWEEN INSTANTANEOUS SURFACE HEAT FLUX, INSTANTANEOUS SURFACE TEMPERATURE, AND TRACKED SHOCK WAVE PHENOMENA.

Investigated are unsteady relationships between surface heat flux variations, surface temperature fluctuations, and tracked shock wave phenomena. The level of coherence and time lag between events at different flow locations are used to quantify the associated interactions at different frequencies. With this approach, time-varying surface heat flux and surface temperature fluctuations are used to track events at different flow locations relative to unsteadiness associated with the test section inlet and relative to unsteadiness associated with different shock wave phenomena. Employed for the investigation is a specialty test section with an inlet Mach number of 1.54, which contains a normal shock wave, a lambda foot (which is comprised of an upstream oblique shock wave leg, and a downstream oblique shock wave leg), and a flow separation zone beneath the lambda foot. High and low unsteady Mach wave intensity levels are produced at the test section inlet by different numbers and different amounts of unsteadiness of families of intersecting and interacting Mach waves, as these are located within and just downstream of the test section entrance. When correlated with respect to normal shock wave tracked locations, values and magnitudes of the most highly correlated frequency bands are different depending upon the level of test section inlet unsteady Mach wave intensity, and the location where unsteady flow events originate. With low freestream unsteady Mach wave intensity at the test section inlet, unsteady events are generally present at normal shockwave locations prior to times when their influences are present at thin film temperature and heat flux gage surface locations. The presence of high unsteady Mach wave intensity at the test section inlet produces an environment wherein the low Mach wave intensity inlet flow is overwhelmed by highly active Mach wave fluctuations, when they are present, such that the normal shock wave is no longer a primary originating source of flow unsteadiness.

RAREFACTION SLIP PHENOMENA WITHIN A VISCOUS DISK PUMP WITH MOLECULAR MEAN FREE PATH SIZED ROUGHNESS ELEMENTES.

Considered are roughness elements which are generally very small relative to the principal flow length scale, and about the same order of magnitude as the molecular mean free path of helium. Significantly different rarefaction flow behavior is produced using three roughness arrangements, which have different character and structure in regard to distributions of larger ridges, and collections of smaller, pointed peaks. Measured distributions of slip velocity and associated tangential momentum accommodation coefficients are provided as they vary with Knudsen number Kn, disk rotation speed, and mean roughness height Ra. Results are given for helium and air as working fluids, three different surface roughness types, different disk rotational speeds, different volumetric flow rates, and different flow passage heights h. Knudsen number values range from $5.21*10^{-3}$ to $2.15*10^{-2}$ for helium, and from $1.82*10^{-3}$ to $7.53*10^{-3}$ for air. The device employed to produce these data is a viscous disk pump (VDP). With smallest mean roughness height, all of the elements on the surface are about the same size, which is about the same as the molecular mean free path of helium, and a larger percentage of molecules are subject to specular reflection resulting in substantial slip velocity magnitudes. With largest mean roughness height, a diversity of roughness element sizes, shapes, and heights is present, and a larger percentage of molecules are subject to diffuse reflection resulting in relatively small slip velocity magnitudes.

INTERRELATIONSHIPS OF ENTROPY PRODUCTION AND TURBULENCE KINETIC ENERGY ASSOCIATED WITH SIMPLE

ANGLE AND COMPOUND ANGLE FULL COVERAGE FILM COOLING.

Compared are experimentally-measured distributions of entropy generation with numerically-predicted distributions of streamwise vorticity, turbulence kinetic energy, and production of turbulence kinetic energy. These comparisons are provided for two full-coverage film cooling environments which are designed to model the thermal management arrangements employed for combustor liners within gas turbine engines. One of these arrangements includes alternating compound angle values of +30 degrees in one row of holes, followed by -30 degrees in the next row of holes. The other arrangement includes simple angle holes with a zero degree compound angle value. The associated full-coverage film cooled boundary layers are investigated within a double-wall cooling test facility wherein the air for each full-coverage film cooling arrangement is provided by an impingement jet array. Experimentally-measured entropy generation values are obtained from film cooled boundary layer measurements of local total pressure variations, obtained in isothermal flow, relative to the freestream values outside of the boundary layer. The resulting entropy generation values quantify second law losses, which are associated with aerodynamic gains. To obtain the associated numerical-prediction results for a steady-state, three-dimensional flow field, employed is the ANSYS FLUENT Version 2022 R2 computational code with a SST k-ω turbulence closure model. The resulting comparisons of entropy generation, streamwise vorticity, turbulence kinetic energy, and production of turbulence kinetic energy are provided for a blowing ratio BR of 2.9 for simple angle film cooling with a main flow Reynolds number Rems of 138,000, and for compound angle film cooling with a main flow Reynolds number Rems of 142,000. Overall, evidence is provided of strong relationships between local turbulence kinetic energy and local entropy production since the two quantities are highly correlated with each other over s substantial range of experimental conditions and configurations. For example, ratio of turbulence kinetic energy to entropy generation data collapse for particular spanwise and normal flow locations, and both film cooling arrangements. Here, the value of the TKE/Sgen ratio is approximately constant for these conditions, which evidences direct and simple dependences of local turbulence kinetic energy upon local entropy generation, even for flow locations close to the test surface. The direct and simple dependences of local turbulence kinetic energy upon local entropy generation are further illustrated by the simplicity of linear correlation equations, which represent physical behavior for different conditions and configurations.

AERODYANMIC LOSSES AND SURFACE HEAT TRANSFER CHARACTERISTICS OF TRANSONIC TURBINE ALLOY BLADES WITH AS-BUILT, MACHINED, ABRASIVE FLOW MACHINED (AFM), AND CHEMICAL AND CHEMICAL MECHANICAL POLISHED (CP+CMP) SURFACES.

As the requirements for rocket engines become more demanding, the additive manufacturing (AM) technique has developed an area of novel alloys, which prove promising for applications in turbines. One such alloy is the NiCoCr based Glenn Research Center Extreme Temperature above 810°C alloy, or GRX-810. This material incorporates the benefits of the AM process as the Yttrium oxide coating of the feedstock powder is evenly dispersed in the component during the laser powder

bed fusion (L-PBF) manufacturing process. A result of this strengthening mechanism is a doubling of the ultimate strength at 1093°C, making GRX-810 components well suited for the high temperature conditions of rocket engine turbines. However, due to the nature of this manufacturing process, post-processing of the components is necessary to achieve desired surface characteristics. Due to a scarcity of research conducted in this field, the present experimental effort aims to investigate the effects of two different surface enhancement techniques, chemical polishing with chemical mechanical polishing and abrasive flow machining, on the aerodynamic losses associated with the flow around a turbine blade and the heat transfer on the blade tip. For this experimental investigation, a two-dimensional linear cascade is used. The linear cascade, consisting of five blades with four flow passages, provides three measurement locations to determine flow parameters. A one-dimensional traverse with a stagnation pressure probe and a calibrated thermocouple $0.25C_x$ downstream of the blade row exit plane is employed to determine aerodynamic loss parameters associated with the flow around the blade profile as the probe sweeps through the wake of the central blade. Spatially-resolved heat transfer data are determined using the impulse response method to provide spatially-resolved surface adiabatic wall temperature data and spatially-resolved surface heat transfer coefficient data. Over large portions of the pressure side, the measured static pressure values for both blades are in close proximity. Diverging behavior is only observed close to the trailing edge, where the flow acceleration along the CP+CMP pressure side is significantly increased. A larger effect of the rougher surface texture of blade CP+CMP on the suction side is also evident in the measurements conducted in the wake downstream of the central blade. The rougher surface texture of the CP+CMP blade is also observed to increase the values of the heat transfer coefficient significantly. Line-averaged heat transfer coefficient data of the blade CP+CMP lies above the values of AFM at every respective location. With the small tip gap channel of 1.4 mm, the higher surface roughness has a decelerating effect on the flow due to larger friction from locally increased surface roughness.

Further Developments in Ion-Solid Interactions

by William J. Weber, Member EUAS

Short Biography

Professor Emeritus, 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 is currently Professor Emeritus in the Department of Materials Science and Engineering at the University of Tennessee. He retired as Professor and Director of the Ion Beam Materials Laboratory in January 2023. From 2010 through 2020, he was the Governor's Chair Professor for Radiation Effects in Materials at the University of Tennessee, 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 MRS Woody White Service Award from the Materials Research Society (2023); the Radiation Effects in Insulators Award from the International Committee on Radiation Effects in Insulators (2023), 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 610journal articles, 118 peer-reviewed conference papers, and 14 book chapters. Based on the Web of Science, his publications have over 30,100 citations, with an h-index of 84; based on Scopus, his publications have over 32,200 citations, with an h-index of 85; based on Goggle Scholar, his publications have over 40,500 citations, with an h-index of 96.

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 high 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. Following thermalization of the electrons and recombination of electrons and holes, a high density of localized electronic defects (trapped electrons, holes and excitons) may remain. 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.

High-entropy ceramics have recently gained recognition for their unique electrical, magnetic, thermal, and optical properties and their potential for diverse applications. The addition of compositional diversity in these ceramic materials (oxides, carbides and borides) with five or more cations on a given lattice site offers the opportunity for property engineering by taking advantage of the high compositional disorder, lattice distortions, mass fluctuation, cation size variations, and integration of diverse cation species. High entropy ceramics have the potential to revolutionize applications in areas such as energy storage, electronics, and photonics, as well as in extreme environments. Ion beam modification provides another opportunity to further tune or pattern the functionalities of high-entropy ceramics; however, little is known about their response to high energy ion beams. At high ion energies (several hundred MeV), amorphous ion tracks, microns in length, are formed along the ion trajectory, creating columnar-like defect structures in high-entropy oxides. At intermediate energies (hundreds of keV to tens of MeV), irradiation-induced defects are introduced and amorphization often occurs in some high-entropy oxides. However, compositional changes can lead to enhanced irradiation resistance in some high-entropy oxides. On the other

hand, high entropy diborides show superior radiation performance compared to quaternary diborides.

Ionoluminescence of strontium titanate ($SrTiO_3$) under the intense electronic excitation produced by 3 MeV H, 19 MeV Si, and 19 MeV Cl ions has been investigated at temperatures ranging from 30 to 100 K. Previously reported emission bands at 2.0 eV, 2.5 eV, and 2.8 eV were observed; furthermore, an asymmetric, narrow emission band centered at 3.15 eV was observed, but only under heavy ion irradiation (19 MeV Si and Cl) at temperatures below 70 K. The nonappearance of the 3.15 eV emission band under irradiation with protons indicates that impurities and any pre-irradiation defect population play a limited role, if any, in the emission process, while higher electronic excitation density is important. In addition, the lack of any fluence-dependent growth in the emission yield indicates that irradiation-induced defects also play a limited role in the emission. Detailed analysis of the proton induced ionoluminescence and heavy ion induced ionoluminescence, as well as available literature on photoluminescence of $SrTiO_3$ at low temperatures photoluminescence of strontium titanate, leads to a conclusion that the 3.15 eV emission is associated with the recombination of large polarons.

It is widely known that the interaction of swift heavy ions with many complex oxides is predominantly governed by the electronic energy loss that creates an intense inelastic thermal spike through electron-phonon coupling along the ion trajectory. This inelastic thermal spike often leads to local melt-quenching processes that result in the formation of nanoscale amorphous ion tracks along the ion trajectory. In order to advance the understanding of the atomic structure of ion tracks, a single crystal wafer of $SrTiO_3$ was irradiated with 629 MeV Xe ions at low fluences to produce isolated amorphous tracks. The atomic-level structure of this irradiated sample was subsequently investigated by comprehensive electron microscopy methods that were complemented by molecular dynamics simulations. The microscopy results revealed discontinuous ion-tracks along the ion trajectories that consisted of an amorphous core and a surrounding shell, only a few monolayers thick, of strained/defective crystalline $SrTiO_3$. Through machine-learning-aided analysis of the atomic-scale images, the presence of 4-8% strain in the disordered shell surrounding the amorphous core of the ion tracks was revealed. Under continuous exposure to the 200 keV electron beam during imaging in the electron microscopy, the amorphous core of the ion tracks was observed to readily undergo radial recrystallization inwardly from the crystalline-amorphous interface. Cation strain in the amorphous region underwent significant recovery; however, the oxygen sublattice remained highly strained under the electron beam due to the presence of oxygen vacancies. The molecular dynamics simulations confirm this observation and

further indicate that local transient heating and annealing facilitate the recrystallization process of the amorphous phase and stimulate the rearrangement of the Sr and Ti sublattices. On the other hand, the recovery of the O sublattice is difficult, and a remnant of oxygen vacancies and strain remain after recrystallization.

The coupled and separate effects of electronic (ionizing) and nuclear (non-ionizing) energy losses on damage evolution in pre-damaged $KTaO_3$ have been investigated by irradiating with intermediate energy O ions (6 MeV, 8 MeV and 12 MeV) at 300 K. The damage evolution was monitored in situ by Rutherford backscattering spectrometry in channeling mode (RBS/C), and the RBS/C results revealed ionization-induced recovery of the pre-damaged state that decreases with increasing O ion energy. These results were confirmed by high resolution transmission electron microscopy analysis. The reduction of the measured disorder level was accompanied by the broadening of the depth profiles of disorder to greater depths with increasing ion fluence, and the results indicated enhanced defect migration with decreasing O ion energy. Since the electronic energy, S_e (~ 3.0 keV nm^{-1}), is nearly constant for all 3 O ion energies across the pre-damaged depth, the difference in recovery and migration behavior is attributed to a "*velocity effect*". Below the Bragg peak in electronic stopping, the velocity of ions is lower, which yields a confined spread of the hot electron cascades that results in an increased energy deposition density. Calculations with the inelastic thermal spike model have further confirmed the existence of a velocity effect on annealing in $KTaO_3$. This effect of ion velocity on ionization-induced annealing has not been rarely reported in other materials. This work advances the understanding of ionization-induced annealing by confirming that ion velocity can affect the healing of pre-existing defects, which may have significant implication for atomic-level control of microstructural modifications in $KTaO_3$ and other materials.

Select Publications Related to This Research

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Hierarchical Metastable Materials: Tuning Phase Formation and Property Optimization

by Jürgen Eckert, Member EUAS

Short Biography

Jürgen Eckert obtained his Ph.D. in Materials Science and Engineering at the Friedrich-Alexander-University Erlangen-Nuremberg, Germany in 1990. 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 was 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. Her also served as Scientific Director of IFW Dresden (2013/2014). In 2015 he became 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 held an Adjunct Professor Position at Michigan Technological University, Houghton, USA (2002-2005), was a Visiting Professor at University of Vienna, Austria (2009/2010/2012) and was appointed Honorary Professor at Shenzhen University, PR China (2021) and Honorary Researcher at Henan Academy of Sciences, Zhengzhou, PR China (2023).

He is an international expert in the field of metastable materials and has published 1390 papers in archival journals (h-index: 108 (WoSci), more than 57.000 citations), as well as more than 150 conference papers, 19 book chapters, 8 edited books, conference proceedings and journal issues, holds 24 patents, and delivered so far more than 265 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 THERMEC Distinguished Award (2023), the European Advanced Materials Award of the International Association of Advanced Materials, Sweden (2021), an ERC-Proof of Concept Grant of the European Research Council (2019), 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 corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences (2017), Member of the European Academy of Sciences (2018), MRS Fellow of the Materials Research Society, USA (2018), Honorary Member of The Indian Institute of Metals, corresponding Member of the Section Technical Sciences of the Saxon Academy of Sciences and Humanities in Leipzig, Germany (2020), Foreign Fellow of the Indian National Academy of Engineering, India (2021), Fellow of the International Association of Advanced Materials (FIAAM), Sweden (2021) and was elected Full Member of Sigma Xi, The Scientific Research Honor Society, USA (2022) and Foreign Fellow of the Indian National Academy of Sciences (NASI), India (2023).

Jürgen Eckert's research activities focus on phase formation and structure-property correlations of metastable materials processed under non-equilibrium conditions; structural and functional materials with particular emphasis on fundamentals of solidification and solid state reactions; additive manufacturing techniques; high strength, biocompatible and magnetic alloys, and materials for sustainable energy applications (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen production and storage) and thin film systems for flexible electronics; 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 seminal contributions in developing metastable advanced high-performance materials. Early work focused on amorphization and quasicrystal formation in metallic systems, and fundamental observations on establishing nanoscale grain sizes in metallic materials. The interest shifted later to the development and property optimization of bulk metallic glasses and composites, high entropy alloys and structurally modulated systems with hierarchically tuned microstructure for creating plastically deformable and tough engineering materials. This work followed a synergistic approach by understanding how atomic scale structures, microstructural features and stress, along with processing-induced heterogeneities determine the mechanisms of plastic deformation on different length scales such as to overcome the otherwise unavoidable brittleness of glassy or nanoscale materials, and evolved into a comprehensive approach using disorder and heterogeneity concepts for creating new strategies to tailor the properties of advanced materials under non-equilibrium conditions. This 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, and touched on surface modification and development of architected gradient structures.

Jürgen Eckert's recent research activities focus on in-depth *in situ* and *in operando* investigations 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) for creating tailored biologically inspired metastable materials with hierarchical structure and tuned disorder. 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 or nanostructured metallic alloys containing heterogeneities on different length-scales to overcome their intrinsic brittleness. The heterogeneities can be triggered through local chemical variations, modulation of short- or medium-range order or via creating locally tuned stress/strain states. The concept of *in-situ* design and testing is applicable to bulk materials, granular or thin film systems and to a variety of materials, and thus opens new research avenues for designing materials with unique properties. Some of the key publications in this area include:

- Q. Xu, X. Yuan, J. Eckert, D. Şopu, "Crack-Healing Mechanism in High-Entropy Alloys under Ion Irradiation", *Acta Mater.* **263**, 119488 (2024).
- S.L. Zhao, B. Jiang, K.K. Song, X.M. Liu, W.Y. Wang, D.K. Si, J.L. Zhang, X.Y Chen, C.S. Zhou, P.P. Liu, D. Chen, Z.Q. Zhang, P. Ramasamy, J.L. Tang, W.Q. Lv, K.G. Prashanth, D. Şopu, J. Eckert, "Machine Learning Assisted Design of High-Entropy Alloys with Ultra-High Microhardness and Unexpected Low Density", *Mater. Des.* **238**, 112634 (2024).
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- C.S. Zhou, Z.D. Kou, K.K. Song, J.H. Gong, P.P. Liu, Q.W. Gao, X.M. Liu, X.L. Han, Z.Q. Zhang, P. Ramasamy, L. Hu, J. Orava, J. Eckert, "Evading Strength-Ductility Trade-Off Dilemma in TRIP-Assisted $Fe_{50}Mn_{30}Co_{10}Cr_{10}$ Duplex High-Entropy Alloys via Flash Annealing and Deep Cryogenic Treatments", *Acta Mater.* **268**, 119779 (2024).
- D. Şopu, X. Yuan, F. Spieckermann, J. Eckert, "Coupling Structural, Chemical and Stress Fluctuations with Relaxation Dynamics in Metallic Glasses", *Acta Mater.* **275**, 120033 (2024).

The long-term perspective of these approaches is to further advance the understanding of structure-property correlations for hierarchically modulated structures and hybrid systems over a variety of different length-scales under highly non-equilibrium thermodynamic and kinetic conditions. The goal is to gain a descriptive and quantitative picture of phase formation, transformation, dynamics, and property design under extreme conditions, such as ultra-fast

heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimulus. Whereas some of these approaches are already followed for crystalline materials, research on disordered and interface dominated materials along these lines touches almost unknown grounds, since the structural diversity represented by disorder in a material represents a holy grail of materials science and promises to overcome the compositional and structural constraints of crystalline materials. The ability to predict and design disorder in architected materials with unique functionality via property-directed material design provides vast opportunities for new structural and functional materials including high-strength-lightweight systems, sustainable and responsive/responsible materials, biomedical implants, or micromechanical components with unique performance characteristics. But not only the fundamental mechanisms of structure formation and property development are of interest, but also the question how the findings can be transferred into parts, devices and systems for MEMS/NEMS, sensor and actuator applications, flexible microelectronics, as well as into materials for energy applications and energy harvesting. Also, biocompatible (biodegradable) bulk materials, porous structures, coatings, and surfaces are in the focus of interest, e.g. for personalized orthopedic implants and medical devices.

For this purpose, state-of-the-art techniques from the fields of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and structure-biological mimetic and 3d printing techniques are used to generate architected materials built from disordered building blocks. Modelling and simulation supplement and strengthen the experimental efforts. Multi-scale modelling techniques based on hierarchies of overlapping scales including quantum mechanics-based structure modelling, atomistic modelling and numerical methods can be involved. A variety of simulation and modelling of length and time scales is utilized, and complemented by Bayesian Interference (BI) and machine learning algorithms to better characterize the local property statistics not assessable with direct measurements. The outcome of this approach allows for both a quantitative parameterization of local properties and protocols by which they are, in general, to be measured. This is a vital input for property-directed and machine learning driven material design of disordered systems, and promises to open new avenues for nanoscale structure formation in architected materials with unique functionality through generating an atomic structural – functional understanding of the properties, performance and correlation of hierarchical thin film structures and membranes, tailored interface structures, nano- and multiscale hybrid systems and tailored lattice materials.

New in Situ Experimental & Theoretical Advances in Severe Plastic Deformations, Strain-induced Phase Transformations & Microstructure Evolution under High Pressure

by Valery I. Levitas, Member EUAS

Short Biography

Valery I. Levitas
Anson Marston Distinguished Professor in Engineering
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Department of Aerospace Engineering & Department of Mechanical Engineering
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Education and Training:
Kiev Polytechnic Institute, Kiev, USSR Mechanical Engineering M.S. (Honors), 1978
Institute for Superhard Materials, Kiev, USSR Materials Science Ph.D., 1981
Ins. Electronic Machinebuilding, Moscow, USSR Continuum Mechanics Dr. of Sci., 1988
University of Hannover, Germany Continuum Mechanics Doctor-Engineer habil., 1995

Appointments

08.08-present *Anson Marston Distinguished Professor in Engineering (2018, permanent); Vance Coffman Faculty Chair Professor (17-), Schafer 2050 Challenge Professor (08-17), Dept. Aerospace Engineering, Dept. Mechanical Engineering; Dept. Material Science and Engineering, Iowa State University; Faculty Scientist, Ames Labor.*

08.02-present *Associate Professor (99-02), Professor (02-08) Lubbock, TX, Department of Mechanical Engineering.*

08.14-12.14 *Visiting Scholar, NIST and Geophysical Lab., Carnegie Institution of Washington.*

01.05-05.05 *Visiting Scholar, Los Alamos National Labs, Los Alamos, NM.*

08.93 -08.99 *Humboldt–Research Fellow (93-95), Visiting & Research Professor (95-99), University of Hannover, Inst. Structural & Computational Mechanics, Hannover, Germany.*

04.78–08.94 *Engineer (78-81), Junior Researcher (81-84), Senior Researcher (84–88), Leading Researcher (89–94); Leader of research group (82–94), Ins. for Superhard Materials of the Ukrainian Academy of Sciences, Kiev, Ukraine.*

Consultant: Los Alamos National Labs; NIST; Geophysical Laboratory, Carnegie Institution of Washington; Ins. for Superhard Materials (Kiev); Seyeon E&S corporation (Daejeon, South Korea).

Products: *483 publications, including 301 refereed journal papers, 3 books, 11 book chapters and 11 patents; 13,832 citations, H-index - 68.*

Selected Awards and Honors

- The best paper of the Journals of Alloys and Compounds award in 2024.
- Board Member of the American Council of the International Association of Advanced Materials (IAAM).
- 2024 ScholarGPS Highly Ranked Scholar in area of Phase Transitions: #5 lifetime and #12 prior

5 years.
- Elected to the European Academy of Sciences and Arts (2023).
- Fellow of the International Association of Advanced Materials (IAAM), Sweden (2023).
- Elected to the EU Academy of Sciences (2022).
- Paper "Levitas V.I. High-Pressure Phase Transformations under Severe Plastic Deformation by Torsion in Rotational Anvils. Material Transactions, 2019, Vol. 60, No. 7, 1294-1301" is recognized as the most cited paper in Material Transactions during 2016-2022.
- Phase transformations and other structural changes in materials: special issue of the International Journal of Plasticity in Honor of Professor Valery I. Levitas; Editorial: Liming Xiong, International Journal of Plasticity, 2021, Vol. 139, 102948. - Symposium on Phase Transformations and other Structural Changes in Materials in honor of Khan's Medal Awardee Prof. Valery Levitas at 25th International Conference on Plasticity, Damage & Fracture 2019, Panama, 1/3/19-1/9/19.
- Khan International Medal Award for outstanding contributions to the field of plasticity (2018).
- Symposium on Structural Changes in Materials in honor of Prof. Valery Levitas at 23rd International Conference on Plasticity, Damage & Fracture 2017, Puerto Vallarta, Mexico, 1/3/17-1/9/17.
- ISU Award for Outstanding Achievement in Research (2016).
- Lifetime Achievement Award for outstanding achievements in engineering, science, and education (Int. Biog. Centre, 2011).
- Honorary Doctor of the Institute for Superhard Materials, Kiev, Ukraine (2011).
- ASME Fellow (2007).
- Barnie E. Rushing Faculty Distinguished Research Award (TTU, 2005).
- Best Professor Award (TTU, Fall'01).
- Richard von Mises Award of GAMM (Society of Applied Mathematics & Mechanics, 1998).
- Int. J. Eng. Sciences Best Paper Award (1995).
Alexander von Humboldt Foundation Fellowship, Germany (1993 – 95, 2012).

New in Situ Experimental & Theoretical Advances in Severe Plastic Deformations, Strain-induced Phase Transformations & Microstructure Evolution under High Pressure

Here, we summarize selected in situ experimental and theoretical studies of coupled severe plastic deformation (SPD), strain-induced phase transformations (PTs), and microstructure evolution under high pressure under compression in diamond anvil cell (DAC) or compression and torsion in rotational diamond anvil cell (RDAC) (Fig. 1) published in 2024.

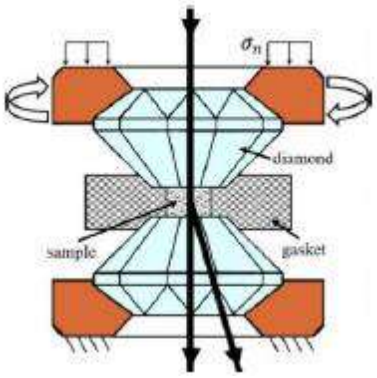

Fig. 1. Schematic of RDAC. Two diamond anvils compress the sample within or without a gasket,

like in traditional DAC, to high pressure. Then torque is applied, leading to the superposition of large shear-dominated straining on compression. The X-ray beam is directed along the axial direction.

1. Plastic strain-induced phase transformations in silicon: drastic reduction of transformation pressures, change in transformation sequence, and particle size effect revealed by in-situ study of Si [1].

Paper [1] reports the first results of an in-situ synchrotron X-ray diffraction (XRD) study of the plastic strain-induced PTs in Si under non-hydrostatic compression in DAC and torsion in RDAC with smooth and rough anvils.

Traditional pressure- and stress-induced PTs between numerous phases of Si, the most important electronic material, have been studied for decades. However, plastic strain-induced PTs are entirely different and promise numerous discoveries. Thus, it was predicted theoretically (opposite to the current theory) that when a reduction in the grain size leads to an increase in the yield strength (Hall-Petch effect) and then to a decrease in the yield strength (inverse Hall-Petch effect), the minimum pressure for strain-induced PT first reduces and then increases. This was confirmed for the appearance of Si-II and is opposite to what we observed in the hydrostatic experiments (Fig. 2). Pressure in small Si-II and Si-III regions was found to be ~5-7 GPa higher than in the parent Si-I. Both results strongly support the suggested mechanism of strain-induced PTs by nucleation at the tip of the dislocation pileup.

For Si powder with an average particle size of 100 nm, strain-induced PT Si-I→Si-II initiates at 0.3 GPa versus 16.2 GPa under hydrostatic conditions (i.e., pressure is reduced by a factor of 54!); for 30 nm Si, it is 4.9 GPa versus ∞, since this PT does not occur at all.

Similarly, strain-induced PT Si-I→Si-III in 100 nm particles initiates at 0.6 GPa, while it does not occur under hydrostatic loading. This minimum pressure is the same for compression in DAC and torsion in RDAC, i.e., it is independent of the plastic strain tensor and its path, which has multiple practical consequences. Also, plastic straining changes the sequence of PTs and leads to the coexistence of four Si phases. Based on the gained understanding, several long-standing puzzles have been resolved: retaining Si-II at ambient pressure and obtaining reverse Si-II→Si-I PT, demonstrating the possibilities of manipulating different synthetic paths. The phase fractions, crystallite size, and pressure in each phase have also been reported for the first time. Single-phase nano Si-III has been obtained in the relatively large region of the sample after compression of 100 nm Si to 11.6 GPa and unloading within several minutes. This contrasts one of the existing techniques, which requires quenching from 14 GPa and 900 K over three days. Nanocomposite of two semiconducting phases Si-I+Si-III in 100 nm Si retained after unloading from 5.2 GPa and rotation by 101.3° may have useful material properties.

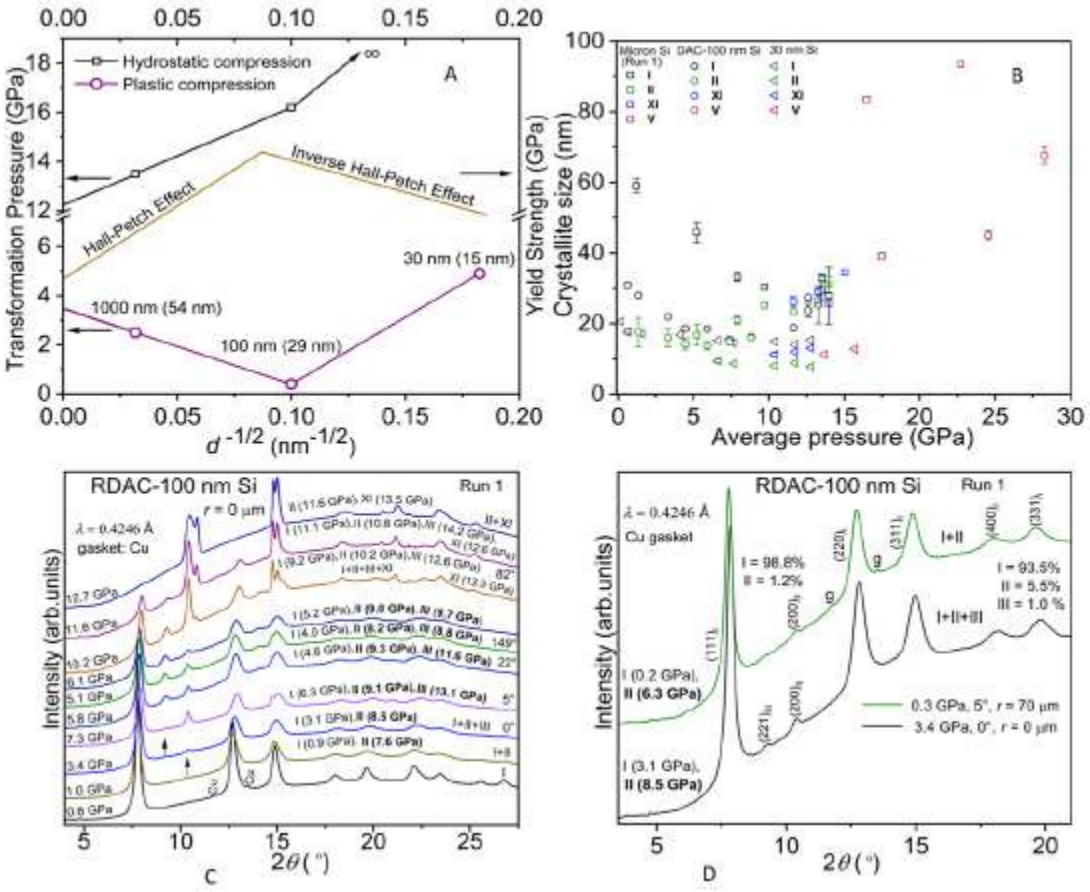

Fig. 2. Selected results on plastic strain-induced phase transformations in silicon [1].

(**A**) Experimental results on particle-size dependence of the minimum Si-I→Si-II PT pressure under plastic straining and hydrostatic loading, and a schematic of particle-size dependence of the yield strength according to the direct and inverse Hall-Petch effects. Numbers in parentheses are crystallite sizes at the initiation of the PT. The correlation between the particle size's direct and inverse Hall-Petch effects on the yield strength and the pressure for strain-induced PT is observed in accordance with the revisited dislocation pileup-based nucleation mechanism. **(B)** The crystallite size *vs*. average pressure in I, II, XI, and V phases of Si for micron, 100 nm, and 30 nm particles are shown as square, circle, and triangle symbols, respectively. **(C)** XRD patterns for 100 nm Si within Cu gasket at various pressures and anvil rotations with smooth diamonds at r = 0 μm. The torsion is applied at 3.4 GPa and 6.1 GPa at r = 0 μm. Pressure in each phase is shown in parentheses. The large pressure values in the Si-II and Si-III compared to Si-I are shown with bold symbols. **(D)** Initiation of Si-I→Si-II PT at 0.3 GPa, r = 70 μm and shear, 5°. The Si-I, Si-II, and Si-III phases coexist at 3.4 GPa, r = 0 μm, and shear, 0°.

Obtained results open new direction in developing the scientific foundation for plastic strain- and defect-induced material synthesis and retrieving the desired nanostructured pure phases or mixture of phases (nanocomposites) with optimal electronic, optical, and mechanical properties. They also challenge the theoretical description of these phenomena.

Reduction in the PT pressures by more than an order of magnitude and their nontrivial scale dependence require serious reconsideration of other engineering problems. Thus, they are important for understanding and optimizing surface treatment (polishing, turning, etc.) of strong brittle semiconductors and ceramics, developing regimes of their ductile machining by promoting PTs to ductile phases, and for friction in NEMS/MEMS. Also, these results warn that some Si phases may appear during surface treatment of Si wafers and friction while they are undesirable.

2. Quantitative kinetic rules for plastic strain-induced α - ω phase transformation in Zr under high pressure [2]

Plastic strain-induced PTs and chemical reactions under high pressure are broadly spread in modern technologies, friction and wear, geophysics, and astrogeology. However, because of very heterogeneous fields of plastic strain $\boldsymbol{E}^p$ and stress $\boldsymbol{\sigma}$ tensors and volume fraction c of phases in a sample compressed in a DAC and impossibility of measurements of $\boldsymbol{\sigma}$ and $\boldsymbol{E}^p$, there are no strict kinetic equations for them. Here, we develop a kinetic model, finite element method (FEM) approach, and combined FEM-experimental approaches to determine all fields in strongly plastically predeformed Zr compressed in DAC, and specific kinetic equation for α-ω PT consistent with experimental data for the entire sample (Fig. 3). Since all fields in the sample are very heterogeneous, data are obtained for numerous complex 7D paths in the space of 3 components of the plastic strain tensor and 4 components of the stress tensor. Kinetic equation depends on accumulated plastic strain (instead of time) and pressure and is independent of plastic strain and deviatoric stress tensors, i.e., it can be applied for various above processes. Our results initiate kinetic studies of strain-induced PTs and provide efforts toward more comprehensive understanding of material behavior in extreme conditions.

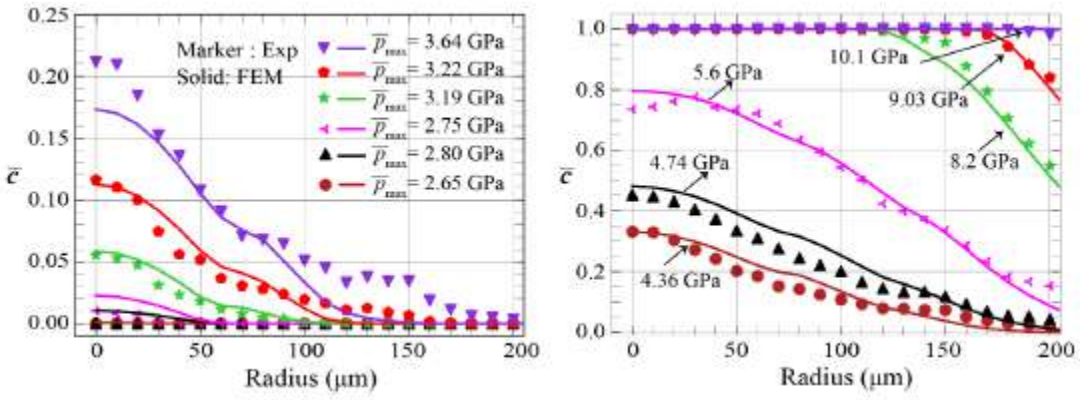

Fig. 3. Comparison of simulated and experimental radial distributions of $\bar{c}$ for the 6 lower and 6 higher loadings marked with averaged through the thickness pressure at the symmetry axis $\bar{p}_{max}$ [2].

3. In situ study of microstructure evolution and α → ω phase transition in annealed and pre-deformed Zr under hydrostatic loading [3].

The detailed study of the effect of the initial microstructure on its evolution under hydrostatic compression before, during, and after the irreversible α→ω phase transformation and during pressure release in Zr using in situ x-ray diffraction is presented. Two samples were studied: one is plastically pre-deformed Zr with saturated hardness and the other is annealed. Phase transformation α→ω initiates at lower pressure for pre-deformed sample but for volume fraction of ω Zr, c>0.7, larger volume fraction is observed for the annealed sample. This implies that the proportionality between the athermal resistance to the transformation and the yield strength in the continuum phase transformation theory is invalid; an advanced version of the theory is outlined.

The crystal domain size significantly reduces, and microstrain and dislocation density increase during loading for both α and ω phases in their single-phase regions (Fig. 4). For the α phase, domain sizes are much smaller for prestrained Zr, while microstrain and dislocation densities are much higher. For the cold rolled sample at 5.9 GPa (just before initiation of transformation), domain size in α Zr decreased to 45 nm and dislocation density increased to 1.1×10^{15} lines/m^2, values similar to those after severe plastic deformation under high pressure. Phenomenological plasticity theory under hydrostatic loading is outlined in terms of microstructural parameters, and plastic strain is estimated. During transformation, the first rule is suggested, i.e., the average domain size, microstrain, and dislocation density in ω Zr for c<0.8 are functions of the volume fraction c of ω Zr only, which are independent of the plastic strain tensor prior to transformation and pressure. The microstructure is not inherited during phase transformation. Surprisingly, for the annealed sample, the final dislocation density and average microstrain after pressure release in the ω phase are larger than for the severely pre-deformed sample.

The significant evolution of the microstructure and its effect on phase transformation demonstrates that their postmortem evaluation does not represent the actual conditions during loading. A simple model for the initiation of the phase transformation involving microstrain is suggested. The results suggest that an extended experimental basis is required for the predictive models for the combined pressure-induced phase transformations and microstructure evolutions.

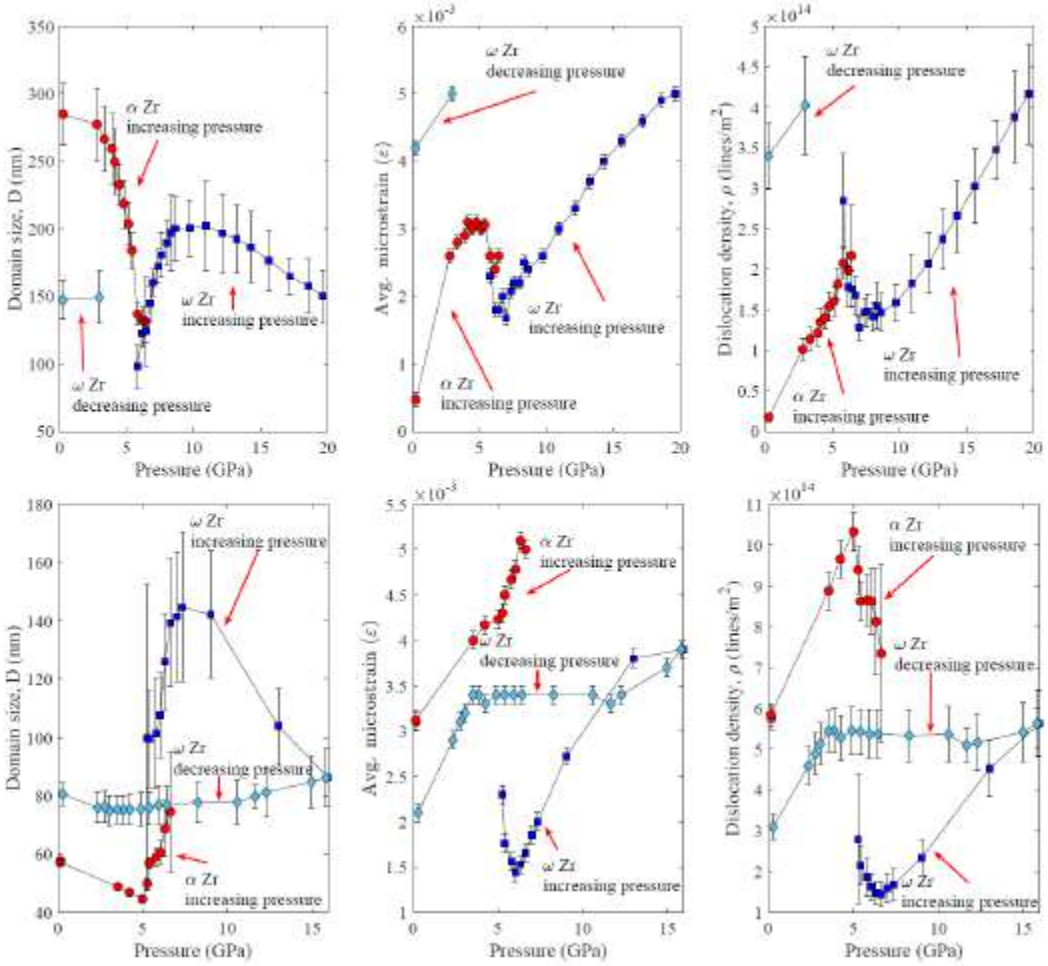

Fig. 4. Average domain size, microstrain, and dislocation density in α and ω Zr for the annealed (top) and cold rolled samples (bottom) while increasing and decreasing pressure [3].

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Toward AI Foundations: An Approach Based on Rough Sets and Interactive Granular Computing (IGrC)

by Andrzej Skowron, Member EUAS

Short Biography

Andrzej Skowron, *ECCAI (EurAI), AAIA and IRSS Fellow, Member of Academia Europaea (MAE), Fellow of the CORE Academy of Sciences and Humanities, Member EU Academy of Sciences, Web Intelligence Academy Founding Fellow (WIA), Advisory Board member of Web Intelligence Consortium, 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 Full Professor in the Systems Research Institute, Polish Academy of Sciences. 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, special issues of journals and volumes of conference proceedings. His areas of expertise include reasoning with incomplete information, approximate reasoning, soft computing methods and applications, rough sets, (interactive) granular computing, intelligent systems, (adaptive) complex systems, perception based computing, machine learning. He was the supervisor of 23 PhD Theses. In the period 1995-2009 he was the Editor-in-Chief of Fundamenta Informaticae journal. He is on Editorial Boards of many others international journals. Andrzej Skowron was the President of the International Rough Set Society (1996-2000). He has delivered numerous invited talks at international conferences. 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 on the ICI Thomson Reuters/ Clarivate Analytics lists of the most cited researchers in Computer Science (globally) in 2012, 2016, 2017. h-index=67 (Google Scholar).*

Abstract

This article is a continuation of Andrzej published articles, particularly in EU ACADEMY ANNUAL REPORTS 2019-2023, and focuses on research work related to Interactive Granular Computing (IGrC) and an approach to rough sets

based on IGrC. More details about IGrC can be found in the papers related to IGrC (see, e.g. [22], papers cited on the website https://dblp.org/pid/s/, and the author's recent invited talks). In this report, we focus on summarization of some main points in an attempt to develop AI foundations for the design and analysis of AI systems aimed at solving problems related to complex phenomena. We propose to use rough sets in the context of IGrC for constructing approximations of concepts, one of the fundamental tasks of approximate reasoning supporting problem solving by AI systems.

Summary of current research aimed at developing AI foundations for building AI systems that solve problems dealing with complex phenomena

The approach is based on a substantial generalization of the existing Granular Computing (GrC) approach (see e.g. [1, 17-19]) and the Rough Set (RS) approach (see e.g. [10, 13-15, 23, 24]). GrC, with information granules as the basic objects, is generalized to Interactive Granular Computing (IGrC) (see, e.g., [5, 6, 21-23]) by introducing complex granules (c-granules), the basic objects of IGrC, which bind abstract and physical objects and make it possible to perceive properties of these objects through c-granules. The IGrC model differs from the classical Turing model. With the IGrC model we try to bring together the issues of language and reasoning as well as action and perception [16]. This research based on IGrC uses existing partial results from different areas such as multi-agent systems, perception and action, machine learning, natural language processing, etc. The IGrC model creates the initial step in developing solid foundations for the design and analysis of AI systems dealing with complex phenomena. The RS approach is generalized by introducing approximation spaces over dynamic networks of granular spaces. Along computations generated over granular networks obtained from granular spaces are discovered entities used through the control of c-granules to discover the relevant computational building blocks for cognition in the form of c-granules or granular networks.

The c-granule control aims to understand the perceived situations for making the right decisions in realizing the specified tasks along the generated granular computations. This is done by discovery of complex games. Any complex game consists of set of rules. The predecessor of any such rule is a classifier for often complex, imprecise and vague concept that triggers specification of transformations appearing on the right side of the rule to be applied to the current granular network when a rule is selected for execution by the c-granule control. The c-granule control's implementation module (IM) is responsible for the physical implementation of specifications of transformations (i.e., the physical semantics). It may be necessary to perform a multi-level decomposition of the specification of transformation to be realized before it can be directly embedded into the physical world.

Complex vague concepts in complex games create one class of concepts to be approximated using the RS approach. Another class consists of concepts in the space of granular computations along which approximate solutions to problems solved by AI systems are constructed. The control mechanism of the c-granule (e.g., corresponding to the constructed AI system) aims at adaptive learning of complex games. This allows c-granules with control to generate computations over granular networks that lead to high-quality approximate solutions, i.e., belonging to the lower approximation of the concept:

high-quality solutions

in the space of granular computations along which these approximate solutions are constructed.

The control of c-granule, supported by its Attention Module (AM), continuously searches the physical world for the perception of relevant data sets represented next in multi-relational approximation spaces or in more general granular spaces and granular networks. The AM uses advanced reasoning techniques, often in collaboration with domain experts. The approximation spaces can be extended to a large family of multi-relational approximation spaces or networks of granular spaces in collaboration with experts, and granular networks are constructed on the basis of them. AI systems perform optimization to identify high-quality complex games. Complex games are adaptively modified based on observed changes in their performance.

In many cases, the AI system represented by c-granule needs to generate the granular computation that leads to the high-quality solutions (relative to the relevant quality measures), even if no known examples of such solutions exist and only some negative examples are available. This is the case, e.g., when the system is searching for new chemical compounds with some specified properties. The success of this generation process depends heavily on the reasoning techniques supporting the c-granule control. The quality of the generated solution (which is determined by the relevant quality measure of the complex game used) often depends on the behavior of this complex game over the entire generated granular computation, not only on its final state.

Information (decision) systems in the RS approach based on IGrC are examples of dynamic information granules whose behavior is considered in the context of the control of the c-granule and is also influenced by interactions from the environment. The universes of objects of information (decision) systems constructed by control of c-granules are formed by expressions satisfying their types represented by formulas expressing properties of fragments of granular computations realized by control of c-granules, which can be stored in information systems.

The approach to RS in the context of IGrC highlights that the approximation problems to be solved by c-granules representing AI systems are significantly more complex than those typically encountered in existing rough-set applications. The success of the control system depends strongly on the quality of both the reasoning techniques and the dialog with domain experts.

This research based on IGrC is important for the realization of a slightly generalized goal of the one formulated in [2]:

> *Tomorrow, I believe,}* [we will use AI SYSTEMS] *to support our decisions in defining our research strategy and specific aims, in managing our experiments, in collecting our results, interpreting our data, in incorporating the findings of others, in disseminating our observations, in extending (generalizing) our experimental observations through exploratory discovery and modeling -- in directions completely unanticipated.*

In the future, we will continue the research on the foundations of IGrC, aiming to extend the current results to societies of c-granules with control as well as their dialogues with experts, chatbots, LLM, and agentic systems.

We will continue our research on the foundations of IGrC with the goal of extending our current findings to societies of c-granules. Designing societies of c-granules with control that provide the desired behavior of them after being combined with another given society of c-granules is a challenge in solving many problems (e.g., discovery of learning algorithms and classifiers, discovery of new medicine or chemical compounds, control of autonomous vehicles, or design of robots [3, 7, 9, 20]).

One of the challenges is to develop the granular deep learning approach based on the IGrC model [12].

Another challenge is to combine the rough set approach based on IGrC with Lifelong Learning (LL) [4]. LL requires techniques to learn in a dynamic and open world or environment in a self-supervised manner, which is consistent with the main goals of IGrC. Many recent applications (e.g., chatbots, self-driving cars, or AI systems interacting with humans/physical environments) need to cope with their dynamic physical and open environments. Therefore, they should continuously learn new things in order to function well. Techniques that support the realization of this goal should be based on the corresponding computational model.

The proposed IGrC model can also be considered as a step towards the realization of the combination of the physical structure and the thinking behavior of the brain. [8]:

> *We should combine the physical structure and thinking behavior of the brain, add physical priors, break through the bottleneck of computing power, realize low-power, low-parameter, high-speed, high-precision, non-depth AI models, and develop more efficient artificial intelligence technology.*

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Local Hormones and Neurolipidomics in Schizophrenia and other Neurological Conditions

by Garth L. Nicolson, Member EUAS

Short Biography

Professor Emeritus Garth L. Nicolson, PhD, MD (H)

Professor Emeritus Garth L. Nicolson is the Founder, President, Chief Scientific Officer and Emeritus Research Professor of Molecular Pathology at the Institute for Molecular Medicine in Huntington Beach, California. He is also a Conjoint Emeritus Professor at the University of Newcastle (Australia). He was previously the David Bruton Jr. Chair in Cancer Research and Professor and Chairman at the University of Texas M.D. Anderson Cancer Center in Houston, and he was Professor of Internal Medicine and Professor of Pathology and Laboratory Medicine at the University of Texas Medical School, Houston. Professor Nicolson has published over 700 medical and scientific papers, including editing 20 books, and he has served on the Editorial Boards of 30 medical and scientific journals and was Senior Editor of four of these. Professor Nicolson has won many awards, such as the Burroughs Wellcome Medal of the Royal Society of Medicine (United Kingdom), Stephen Paget Award of the Metastasis Research Society, U.S. National Cancer Institute Outstanding Investigator Award, the Innovative Medicine Award of Canada and the EU Academy of Sciences. He is also a Colonel (O6, Honorary) of the U. S. Army Special Forces and a U.S. Navy SEAL (Honorary) for his work on Armed Forces and veterans' illnesses.

Professional Experience:

Primary Appointment:

1996-Present, President and Founder, Chief Scientific Officer and Emeritus Professor of MolecularPathology, The Institute for Molecular Medicine, PO Box 9355, S. Laguna Beach, CA 92652

Secondary Appointments:

2003-Present, Conjoint Emeritus Professor, Faculty of Science and Technology, University of Newcastle, Newcastle, Australia

Previous Appointments:

1989-00, Professor, Department of Internal Medicine, The University of Texas Medical School, Houston, TX
1981-99, Adjunct Professor, Department of Pathology, School of Veterinary Medicine, Texas A & M University, College Station, TX
1982-99, Professor, Department of Pathology and Laboratory Medicine, The University of Texas Medical School, Houston, TX
1980-96, David Bruton Jr. Chair in Cancer Research, Professor and Chairman, Tumor Biology, The University of Texas M. D. Anderson Cancer Center, Houston, TX
1980-96, Professor, The Graduate School of Biomedical Sciences, The University of Texas Health Science Center, Houston, TX
1980-87, Florence M. Thomas Professor of Cancer Research, The University of Texas M. D. Anderson Cancer Center, Houston, TX
1978-80, Professor, Department of Physiology and Biophysics, College of Medicine, University of California, Irvine, CA
1977-80, Associate Director, Oncology Program, University of California, Irvine, CA
1975-80, Professor, Department of Developmental and Cell Biology, University of California, Irvine
1974-76, Chairman, Department of Cancer Biology, The Salk Institute, La Jolla, CA
1972-74, Head, Cancer Council Laboratory, Director, Electron Microscopy Laboratory, The Salk Institute, La Jolla, CA
1970-71, Senior Research Associate, Cancer Council Laboratory, The Salk Institute, La Jolla, CA
1967-70, USPHS Predoctoral Fellow University of California, San Diego, CA

Honors and Awards:

European Union Academy of Sciences, 2019-
Doctor of Medicine, M.D. (H), University of the Republic of Uruguay, 2015
Yanagimachi Distinguished Lectureship, University of Hawaii School of Medicine, 2012
John Drulle Memorial Lectureship, International Lyme and Associated Diseases Society (ILADS), 2008

Annual Award of the Common Cause Medical Research Foundation (Canada), 2006
Innovative Medicine Award (Canada), 2002
Stephen Paget Award, Metastasis Research Society, 1998
Albert Schweitzer Award (Portugal), 1998
First Norman N. Durham Lectureship, Environmental Institute, OSU, 1996
Indo-American Society for Health & Laboratory Professionals Award, 1996
Distinguished Presentation Award, Third International Cancer Molecular Biology Symposium, 1996
COLONEL (Honorary), U. S. Army Special Forces, 1995
SEAL (Honorary), U.S. Navy Special Forces, 1995
Haskel Visiting Professorship, University of Pennsylvania, 1995
Burroughs Wellcome Medal, Royal Society of Medicine Foundation, London, 1991
Outstanding Faculty Award, The University of Texas Health Science Center at Houston, 1991
U.S. National Cancer Institute U.S.S.R. Scientist Exchange Award for Collaborative Research on Molecular and Genetic Aspects of Tumor Metastasis, 1991
Evan and Marion Helfaer Distinguished Lectureship, The Cancer Center of the Medical College of Wisconsin, 1990
Dean's Teaching Excellence List, The University of Texas Health Science Center at Houston Graduate School of Biomedical Sciences, 1985-1994
Teaching Excellence Award for Best Course, The University of Texas Medical School at Houston, 1990
NCI/NIH Outstanding Investigator Award, 1987
Annual Award of the Japan Histochemical Society, 1976
Eli Nadel Memorial Lecture in Biochemistry, 1983
Rita Ferdinand Memorial Lectureship, 1982
Guy Lipscomb Memorial Lecture in Chemistry, 1980
Upjohn Biology Education Award, 1976
Presidential Award, Electron Microscopy Society of America, 1971

Progress Report 2024

1. Local hormones and neurolipidomics in schizophrenia and other neurological conditions.

Publication: Sfera, A., Hazan, S., Bota, P.G., Anton, J.J. and Nicolson, G.L. Local hormones and neurolipidomics in schizophrenia. Am. J. Neurol. Res., 2(2): 1-4 (2024).

Most patients with schizophrenia (SCZ) do not exhibit violent behaviors and are more likely to be victims rather than perpetrators of violent acts. However, a subgroup of forensic detainees with SCZ exhibit tendencies to engage in criminal violations. Although numerous models have been proposed, ranging from substance use, serotonin transporter gene, and cognitive dysfunction, the molecular underpinnings of violence in SCZ patients remains elusive. Lithium and clozapine have established anti-aggression properties and recent studies have linked low cholesterol levels and ultraviolet (UV) radiation with human aggression, while vitamin D3 reduces violent behaviors. A recent study found that vitamin D3, omega-3 fatty acids, magnesium, and zinc lower aggression in forensic population. Here we take a closer look at aryl hydrocarbon receptor (AhR) and the dysfunctional lipidome in neuronal membranes, with emphasis on cholesterol and vitamin D3 depletion, as sources of aggressive behavior. We also discuss modalities to increase the fluidity of neuronal double layer via membrane lipid replacement

(MLR) and natural or synthetic compounds.

2. Membrane Lipid Replacement for reconstituting mitochondrial function and—moderating cancer-related fatigue, pain and other symptoms while counteracting the adverse effects of cancer cytotoxic therapy.

Publication: Nicolson, G.L. and Ferreira de Mattos, G. Membrane Lipid Replacement for reconstituting mitochondrial function and moderating cancer-related fatigue, pain and other symptoms while counteracting the adverse effects of cancer cytotoxic therapy. Clin. Expl. Metastasis 41: 199-217 (2024).

Cancer-related fatigue, pain, gastrointestinal and other symptoms are among the most familiar complaints in practically every type and stage of cancer, especially metastatic cancers. Such symptoms are also related to cancer oxidative stress and the damage instigated by cancer cytotoxic therapies to cellular membranes, especially mitochondrial membranes. Cancer cytotoxic therapies (chemotherapy and radiotherapy) often cause adverse symptoms and induce patients to terminate their anti-neoplastic regimens. Cancer-related fatigue, pain and other symptoms and the adverse effects of cancer cytotoxic therapies can be safely moderated with oral Membrane Lipid Replacement (MLR) glycerolphospholipids and mitochondrial cofactors, such as coenzyme Q_{10}. MLR provides essential membrane lipids and precursors to maintain mitochondrial and other cellular membrane functions and reduce fatigue, pain, gastrointestinal, inflammation and other symptoms. In addition, patients with a variety of chronic symptoms benefit from MLR supplements, and MLR also has the ability to enhance the bioavailability of nutrients and slowly remove toxic, hydrophobic molecules from cells and tissues.

3. Role of mycoplasmal infections in fatiguing illnesses: chronic fatigue and fibromyalgia syndromes, Gulf War illnesses and rheumatoid arthritis

Publication: Nicolson, G.L., Nasralla, M.Y., Franco, A.R., De Meirleir, K., Nicolson, N.L., Ngwenya, R. and Haier, J. Role of mycoplasmal infections in fatiguing illnesses: chronic fatigue and fibromyalgia syndromes, Gulf War Illness and rheumatoid arthritis. In: Chronic Fatigue Syndrome: critical reviews and clinical advances: what does the research say? Eds. Montero, R.P. and De Meirleir, K., Taylor & Francis (2024)

Bacterial and viral infections are associated with several fatigue illnesses, including Chronic Fatigue Syndrome (CFS), Fibromyalgia Syndrome (FMS), Gulf War Illnesses (GWI) and Rheumatoid Arthritis (RA), as causative agents, cofactors or

opportunistic infections. We and others have looked for the presence of invasive pathogenic mycoplasmal infections in patients with CFS, FMS, GWI and RA and have found significantly more mycoplasmal infections in CFS, FMS, GWI and RA patients than in healthy controls. Most patients had multiple mycoplasmal infections (more than one species). Patients with chronic fatigue as a major sign often have different clinical diagnoses but display overlapping signs/symptoms similar to many of those found in CFS/FMS. When a chronic fatigue illness, such as GWI, spreads to immediate family members, they present with similar signs/symptoms and mycoplasmal infections. CFS/FMS/GWI patients with mycoplasmal infections generally respond to particular antibiotics (doxycycline, minocycline, ciprofloxacin, azithromycin and clarithromycin), and their long-term administration plus nutritional support, immune enhancement and other supplements appear to be necessary for recovery. Examination of the efficacy of antibiotics in recovery of chronic illness patients reveals that the majority of mycoplasma-positive patients respond and many eventually recover. Other chronic infections, such as viral infections, may also be involved in various chronic fatigue illnesses with or without mycoplasmal and other bacterial infections, and these multiple infections could be important in causing patient morbidity and difficulties in treating these illnesses.

4. Membrane Lipid Replacement and its role in restoring mitochondrial membrane function and reducing symptoms in aging and age-related clinical conditions.

Publication: Nicolson, G.L., Ferreira de Mattos, G., Settineri, R. and Breeding, P.C. Membrane Lipid Replacement and its role in restoring mitochondrial membrane function and reducing symptoms in aging and age-related clinical conditions. Nature Cell Sci. In press (2025).

Aging is a multifaceted, dynamic process—at the subcellular level it involves mitochondrial and nuclear structures as well as metabolic, inflammatory, and signaling processes that result in progressive declines in cellular, organ, and tissue functions, resulting in a greater risk of age-associated morbidity and mortality. Here we focus on the importance of free radical oxidant modifications of membranes that result in the loss of mitochondrial membrane and other organelle membrane functions that are due, in part, to a decline in mitochondrial inner membrane transmembrane potential ($\Delta\Psi_m$). Mitochondrial inner membranes (as well as other cellular membranes) can be repaired, and transmembrane potential restored with Membrane Lipid Replacement, the use of dietary supplements containing protected, undamaged, functional membrane glycerophospholipids that remove and replace damaged membrane phospholipids that build up during normal aging and in several acute and chronic clinical conditions. In particular, reductions in mitochondrial function and heightened membrane damage can result in a variety of symptoms or multi-morbidities found in essentially all age-related chronic

conditions and in diseases where cytotoxic treatments are used, such as cancer cytotoxic therapies. Clinical studies have shown that protected membrane phospholipid supplements can restore mitochondrial and other cellular membranes, resulting in recovery of function and decreases in pain, fatigue, gastrointestinal, and other symptoms in aged individuals and in patients expressing a variety of morbidities. The same supplements can also be used to safely remove toxic hydrophobic chemicals from tissues and cells, providing an effective substitute or addition to pharmaceuticals for age-related illnesses and conditions.

5. The LINC complex in blood vessels: from physiology to pathological implications in arterioles.

Publication: Ferreira, G., Cardozo, R., Chavarria, L., Santander, A., Sobrevia, L., Chang, W. and Nicolson, G.L. The LINC complex in blood vessels: from physiology to pathological implications in arterioles. J. Physiology, in press (2025).

The LINC (Linker of Nucleoskeleton and Cytoskeleton) complex is a critical component of the cellular architecture that bridges the nucleoskeleton and cytoskeleton and mediates mechanotransduction to and from the nucleus. Though it plays important roles in all blood vessels, it is in arterioles that this complex plays a pivotal role in maintaining endothelial cell integrity, regulating vascular tone, forming new microvessels, and modulating responses to mechanical and biochemical stimuli. It is also important in vascular smooth muscle cells and fibroblasts, where it possibly plays a role in the contractile to secretory phenotypic transformation during atherosclerosis and vascular aging, and in the migration and inflammatory responses of fibroblasts in the adventitia. Physiologically, the LINC complex contributes to the stability of arteriolar structure, adaptations to changes in blood flow, and injury repair mechanisms. Pathologically, dysregulation or mutations in LINC complex components can lead to compromised endothelial function, vascular remodeling, and exacerbation of cardiovascular diseases such as atherosclerosis (arteriolosclerosis). This review synthesizes our current understanding of the roles of the LINC complex in cells from arterioles, highlighting its physiological functions, exploring its implications for vascular pathology, and emphasizing its role in endothelial cells. By elucidating the LINC complex's role in health and disease, we aim to provide insights that could improve future therapeutic strategies targeting LINC complex-related vascular disorders.

6. A simple and safe method to slowly remove hydrophobic aliphatic hydrocarbons from petrochemically exposed patieints using an oral Membrane Lipid Replacement natural oral lipid supplement.

Publication: Nicolson, G.L. A simple and safe method to slowly remove

hydrophobic aliphatic hydrocarbons from petrochemically exposed patieints using an oral Membrane Lipid Replacement natural oral lipid supplement. Univ. J. Petroleum Sci. submitted (2025).

Exposures to aliphatic hydrocarbons and polycyclic aromatic hydrocarbons and their heat-generated fragments during the Persian Gulf War in 1991 resulted in long-term symptoms of chemical contamination in deployed armed forces. Some of the veterans display to this day a variety of signs and symptoms related to such exposures. With our success in using oral Membrane Lipid Replacement (MLR) therapy to repair and enhance mitochondrial function and slowly remove oxidized, amphipathic lipids from cellular stores we undertook a study to see if chemically exposed veterans of the Gulf War could benefit from MLR in terms of slowly resolving various chronic signs and symptoms. After 6 months on 6 grams per day oral MLR glycerophospholipids veterans with chemical exposures showed significant reductions in signs and symptoms related to fatigue, pain, chemical sensitivities, neurologic symptoms, gastrointestinal symptoms, breathing, skin lesions and other signs and symptoms. Reductions in the severities of signs and symptoms were gradual and varied among the male subjects in this study. There were also no adverse events during the study. We propose that MLR with protected membrane glycerophospholipids is a simple and safe method to detoxify petrochemical and other hydrophobic toxic chemicals in patients with chronic signs and symptoms.

Integral and Inverse Reinforcement Learning for Optimal Control Systems and Games

by Frank Lewis, Member EUAS

Short Biography

Dr. Frank L. 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 moved to UTA in 1990. He is Moncrief-O'Donnell Endowed Chair Professor of Electrical Engineering at The University of Texas at Arlington.

Ranked #1 scholar in the world in Optimal control, #1 in Reinforcement learning, #2 in Control theory, #4 in Neural networks, #8 in Intelligent control, #14 in Multi-agent systems. Google Scholar page is

https://scholar.google.com/citations?user=rMRit3UAAAAJ&hl=en&oi=sra

Lewis is Ranked as number 24 of all scientists in the world and 12 in the USA in Electronics and Electrical Engineering by Research.com. Ranked number 5 in the world in the subfield of Industrial Engineering and Automation according to a Stanford University Research Study in 2021.

Awarded Top 10 Inspiring Leaders of 2024 by Impact Entrepreneur Magazine.

Recognized as a Top 1% Highly Top Cited Researcher by Clarivate Web of Science every year during 2019-2024. **

Graduated 60 PhD students. Fellow, National Academy of Inventors. Life Fellow of the IEEE, Fellow of IFAC, Fellow of the U.K. Institute of Measurement & Control, Fellow European Union Academy of Sciences, 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. Published 527 Refereed Journal Papers. 104,317 google citations, h-index 140. Published 35 books. Awarded 8 US Patents. 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 Fulbright Fellow Professor at Democritus University in Greece. Invited for research visits at 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, numerous International 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, AI Artificial Intelligence. Nonlinear systems, intelligent control, process control, and neurobiological systems. Received 8 U.S. patents, Wrote 527 journal papers, 52 chapters and encyclopedia articles, 420 refereed conference papers, and 35 books including the internationally acclaimed textbooks 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 $17 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.

1. Directed Graph Clustering Algorithms, Topology, and Weak Links

IEEE TRANSACTIONS ON SYSTEMS, MAN, AND CYBERNETICS: SYSTEMS, VOL. 52, NO. 6, JUNE 2022, 3995-4009.

Xiao Zhang, Bosen Lian, Frank L. Lewis, Yan Wan and Daizhan Cheng

Abtract

In this article, a general approach for directed graph clustering and two new density-based clustering objectives are presented. First, using an equivalence between the clustering objective functions and a trace maximization expression, the directed graph clustering objectives are converted into the corresponding weighted kernel *k*-means problems. Then, a nonspectral algorithm, which covers both the direction and weight
information of the directed graphs, is thus proposed. Next, with Rayleigh's quotient, the upper and lower bounds of clustering objectives are obtained. After that, we introduce a new definition of weak links to characterize the effectiveness of clustering. Finally, illustrative examples are given to demonstrate effectiveness of the results. This article provides a glance at the potential connection between density-based and pattern-based clustering. Compared with other approaches for

directed graph clustering, the method proposed in this article naturally avoids the loss of the nonsymmetric edge data because there is no need for any additional symmetrization.

2. Leader-following consensus of a class of heterogeneous uncertain multi-agent systems with a distributed model reference adaptive control law

Int J Adapt Control Signal Process. 2023;37:1582–1591.

MaryamNicole Naleini, Ahmet Taha Koru, Frank L. Lewis

Abtract

This paper considers the leader-following consensus problem of a multi-agent system whose agents have heterogeneous uncertain dynamics in homogeneousstate dimensions. Each agent utilizes a distributed model reference adaptive control (MRAC) law to deal with uncertainties. The nominal part of the MRAC is a distributed static state feedback control law. The reference model is the leader-following consensus problem of reference agents with homogeneous linear time-invariant dynamics. This problem becomes an N-player graphical differential game under a given cost function. The reference agents utilize distributed static state feedback controllers that constitute a Nash equilibrium solution to the graphical differential game. This paper provides the conditions for the distributed MRAC to guarantee that each agent asymptotically tracks the corresponding reference agent; consequently, the multi-agent system solves the leader-following consensus problem as the reference model does. These conditions yield a straightforward design method for theMRAC.A numerical example demonstrates an application of the proposed approach to a multi-robot system with nonlinear dynamics.

3. Integral and Inverse Reinforcement Learning for Optimal Control Systems and Games

Advances in Industrial Control, 2023 - Monograph

Bosen Lian · Wenqian Xue · Frank L. Lewis · Hamidreza Modares · Bahare Kiumarsi

Control engineering is considered rather differently by researchers who often produce very general design approaches and engineers who must implement and maintain specific industrial control systems. It is of course valuable to develop algorithms for control problems with a well-defined mathematical basis, but engineers often have different concerns over the limitations of equipment, quality of control, safety, security, and possible system downtime. The monograph series

Advances in Indus-trial Control (AIC) attempts to bridge this divide by encouraging the consideration of advanced control techniques where they offer real benefits and where they also address some of the more practical everyday problems.

The rapid development of new control theory, techniques, and technology has an impact on all areas of engineering. This series focuses on applications of advanced control that may even stimulate the development of new industrial control paradigms. This is desirable if the different aspects of the "control design" problem are to be explored with the same dedication that "analysis and synthesis" problems have received in the past. The series enables researchers to introduce new ideas moti-vated by challenging problems in interesting applications. It raises awareness of the various benefits that advanced control can provide whilst also covering the chal-lenges that can arise. This monograph has the role of introducing the state of the art in the exciting and rapidly expanding area of artificial intelligence—(AI)-based, data-driven control.

This monograph for the series is concerned with "reinforcement learning and inverse reinforcement learning" for "optimal" control systems. This is one of the most useful areas for AI to be employed in control engineering applications. Reinforcement learning is based on the simple idea that animals adapt their behaviour based on rewards or punishments received. Chapter 1 introduces the ideas of reinforcement learning and integral reinforcement learning (IRL) with a view to reducing steady-state errors. Inverse reinforcement learning is the inverse problem of reinforcement learning, i.e., the problem of inferring the "reward function" of an expert or agent, given its policy, or observed behaviour, and without prior knowledge of the system model. The subject has much in common with a general form of adaptive control, and indeed, a family of optimal adaptive controllers can be developed using traditional reinforcement-learning methods.

Chapter 2 discusses several areas of optimal control that are reasonably well-known but these are needed for later use. It begins with the topic of IRL using linear quadratic regulator (LQR) ideas. Chapter 3 concerns optimal regulation problems. IRL for optimal regulation problems provides a type of adaptive controller. These can learn about the systems dynamics in the absence of complete plant knowledge and they enable the online learning of the optimal gains in real time.

Chapter 4 considers IRL for optimal control-based tracking problems. The design approach provides optimal tracking performance and at the same time allows system constraints to be satisfied. The combination with the very well-known and familiar linear quadratic optimal control philosophy is helpful since it makes the material on "learning policy" easier to understand.

Chapter 5 considers IRL for "zero-sum games" (where the sum of the amounts won equals the combined losses of other players). This is a useful approach for the solution of upper H Subscript normal infinityoptimal tracking control problems. Unlike the usual upper H Subscript normal infinityoptimal control problems where the system dynamics are assumed to be known, in this case, robust controllers can be found to handle disturbances and uncertainties in the system dynamics.

In Part II of the text the problem of "inverse reinforcement learning" for optimal control systems is discussed. Inverse reinforcement learning infers the implicit

reward function or cost function from the behaviour experienced. Given the reward function and a system model, an optimal controller can, of course, be computed. Chapter 6 begins with reinforcement learning for LQRs assuming no external distur-bances. Both model-based and model-free data-driven inverse reinforcement learning algorithms are described along with their properties.

Chapter 7 deals with systems that have noncooperative and adversarial inputs such as disturbances. The optimal control solution is obtained by minimizing the effects of the worst-case adversarial input, using the Hamilton–Jacobi–Isaacs equation for nonlinear systems or the usual game algebraic Riccati equation for linear systems. The focus is on model-free inverse solutions for dynamic systems.

Chapter 8 turns to the more difficult problem of inverse reinforcement learning for multiplayer non-zero-sum games. There is a range of applications that involve multiple control inputs, such as in road vehicles, where there are various controls (steering wheel, pedals for acceleration and braking, turning signals, and gear selectors).

This text necessarily involves significant theoretical analysis and synthesis theory, but the results provided have a rather practical aim. The theoretical problems and solutions are probably the simplest that could be chosen to illustrate the potential of the algorithms developed. The aim to reduce dependency on models and rely more on data obtained for the control design process is quite challenging. The need to improve the quality of control through learning is also an ambitious target.

The text includes simulation examples in the chapters to illustrate the ideas and it has a set of references and an appendix to help the reader.

The monograph is very suitable for students and researchers working on the use of AI in control systems since it provides a mathematical basis in an area where ideas are often presented in an intuitive style. Engineers wishing to use AI and machine learning methods in areas such as robotics, automotive applications, aircraft systems, power systems, and chemical processes can be comforted that the approach described in this AIC monograph is relatively simple given the challenge and complexity of the problem.

Improvements in Radiative Heat Transfer, the Energy Transfer by Infrared or Electromagnetic Waves

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 Professor Emeritus of Tohoku University
2017- 2023 President, National Institute of Technology, Hachinohe College
2023 Professor Emeritus of 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
HTSJ Honorary Member, 2020

Research Activities

Professor Shigenao Maruyama specializes in thermal engineering. He has published more than 10 books and 300 academic research papers, and has acquired 60 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].

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Improved Modeling of Fluid Flow in Porous Media

by Russell Johns, Member EUAS

Short Biography

Russell T. Johns is the George E. Trimble Chair of Energy and Mineral Sciences at the Department of Energy and Mineral Engineering at Penn State. He recently served as interim head of the John and Willie Leone Family Department of Energy and Mineral Engineering from 2023 – 2024, managing over 60 faculty, 10 staff, and 1000 affiliated undergraduate and graduate students. Prior to that, he served as Chair of the Petroleum and Natural Gas Engineering Program from 2015 to 2018, Distinguished SPE Lecturer for 2019–2020, and Editor-In-Chief for all SPE technical journals from 2018–2020. He was director of the Enhanced Oil Recovery consortium in the EMS Energy Institute at Penn State until 2020.

Before his current position at Penn State, he served on the petroleum engineering faculty at The University of Texas at Austin from 1995 to 2010. He also has nine years of industrial experience as a petrophysical engineer with Shell Oil and as a hydrogeologist for Colenco Power Consulting in Baden, Switzerland. He holds a B.S. degree in electrical engineering from Northwestern University and M.S. and Ph.D. degrees in petroleum engineering and water resources from Stanford University. He has over 250 publications in enhanced oil recovery, thermodynamics, and phase behavior, unconventional gas engineering, multiphase flow in porous media, and well testing. Johns received the SPE Ferguson medal in 1993, the Society of Petroleum Engineers (SPE) Distinguished Member award in 2009, the SPE Faculty Pipeline award in 2013, the 2016 SPE international award in Reservoir Description and Dynamics, the Wilson Excellence in Research award from the College of Earth and Mineral Sciences in 2018, the prestigious IOR Pioneer Award from SPE in 2022, and the highest technical award from SPE in 2023, the Anthony F. Lucas Gold medal.

The research group of Dr. Johns is noted for its development of the first flash calculation algorithm for microemulsion phases where all Winsor regions (single, two, and three-phase) are modelled simultaneously. His group is also recently recognized as developing state function theory of relative permeability to fit experimental data and predict relative permeabilities away from that data set. As a part of that research, they developed an analytical function that includes connectivity (Euler number) in the relative permeability model. Finally, his group has been recognized as a leader in developing miscibility theory for gas injection applications such as injection of carbon dioxide into oil reservoirs. They developed analytical theory for solving hyperbolic equations to predict the minimum miscibility pressure (MMP) for any number of components.

Dr. Johns currently teaches a required undergraduate course in advanced reservoir dynamics, along with a required graduate course in energy thermodynamics, which couples phase behavior and chemical reactions. He also teaches elective graduate courses in gas and chemical flooding for enhanced oil recovery. He is a member of numerous Penn State and professional committees. Selected abstracts from publications this year from his group are included below, along with a brief publication list.

Reliable Equivalent Alkane Carbon Number Determination for Dead and Live Crudes in Microemulsion Systems

Yoga, H.F., Gasimli, N.R., and Johns, R.T., *SPEJ* (2024)

Abstract

A successful surfactant flood maximizes oil recovery by achieving ultralow oil/water interfacial tension (IFT) at the optimal salinity (S*). Optimal salinity, among other parameters, is dependent on the equivalent alkane carbon number (EACN) of the oil pseudocomponent. In this paper, we compare common EACN determination methods used for dead crude at ambient pressure and then propose a third more consistent and reliable method that simultaneously fits data from both methods. The first method is based on a linear plot of lnS* and EACN of pure alkanes, where the dead crude EACN is linearly interpolated using the measured lnS* of the crude. The second method determines the crude EACN by iteration until the measured lnS* of the dead crude and all dilution measurements become nearly linear. For live oil, the EACN is based on the common linear EACN mixing rule but corrected for pressure.

The results show that inconsistencies in estimated crude EACN using the common two methods are resolved when regression is made on all data simultaneously and when an unbiased estimate of optimal salinity is made using hydrophilic-lipophilic deviation–net average curvature (HLD-NAC) theory, where the inverse of three-phase solubility is linear with lnS*. No nonlinear behavior, as has been reported in the literature using the same data, is observed when fit this way and using the simple graphical approach. The graphical approach determines the optimal salinity based on the intersection of the linear regressions of inverse oil and water solubility with lnS*. This approach has the advantage that the optimum is unbiased, and its uncertainty is easily estimated. Using a combination of ambient and high-pressure data, we also show that the EACN of the live oil can be estimated using a methane alkane carbon number (ACN) of 1.0, as it should physically be, when the effect of pressure is properly included.

Fluid-Fluid Interfacial Area and Its Impact on Relative Permeability: A Pore Network Modeling Study

Mukherjee, S., Johns, R.T., Foroughi, S., and Blunt, M.J., *SPEJ* (2023)

Abstract

Relative permeability (k_r) is commonly modeled as an empirical function of phase saturation. Although current empirical models can provide a good match of one or

two measured relative permeabilities using saturation alone, they are unable to predict relative permeabilities well when there is hysteresis or when physical properties such as wettability change. Further, current models often result in relative permeability discontinuities that can cause convergence and accuracy problems in simulation. To overcome these problems, recent research has modeled relative permeability as a state function of both saturation (*S*) and phase connectivity (*X*). Pore network modeling (PNM) data, however, show small differences in relative permeability for the same *S*-*X* value when approached from a different flow direction. This paper examines the impact of one additional Minkowski parameter (Mecke and Arns 2005), the fluid-fluid interfacial area, on relative permeability to identify if that satisfactorily explains this discrepancy.

We calculate the total fluid-fluid interfacial areas (*IA*) during two-phase (oil/water) flow in porous media using PNM. The area is calculated from PNM simulations using the areas associated with corners and throats in pore elements of different shapes. The pore network is modeled after a Bentheimer sandstone, using square, triangular prism, and circular pore shapes. Simulations were conducted for numerous primary drainage (PD) and imbibition cycles at a constant contact angle of 0° for the wetting phase. Simultaneous measurements of capillary pressure, relative permeability, saturation, and phase connectivity are made for each displacement. The fluid-fluid IA is calculated from the PNM capillary pressure, the fluid location in the pore elements, and the pore element dimensional data.

The results show that differences in the relative permeability at the same (*S, X*) point are explained well by differences in the fluid-fluid interfacial area (*IA*). That is, for a larger change in *IA* at these intersection points, the permeability difference is greater. That difference in relative permeability approaches zero as the difference in *IA* approaches zero. This confirms that relative permeability can be modeled better as a unique function of *S, X*, and *IA*. The results also show that an increase in *IA* restricts flow decreasing the nonwetting (oil) phase permeability. This decrease is caused by an increase in the throat area fraction compared to the corner area as the total area *IA* increases. The wetting phase relative permeability, however, shows the inverse trend in that its relative permeability is greater when *IA* becomes larger owing to a greater fraction of the total area associated with the corners. The area *IA*, however, impacts the nonwetting phase relative permeability more than the wetting phase relative permeability. Corner flow improves the wetting phase relative permeability because the wetting phase is continuous there. Finally, a sensitivity analysis shows that relative permeability is more sensitive to change in *S* than it is for *IA* for the case studied, implying that if only two parameters are used to model relative permeability, it is better to choose *S* and *X*.

Comparative Study of Traditional and Deep-Learning Denoising Approaches for Image-Based Petrophysical Characterization of Porous Media

Tawfik, M.S., Adishesha, A.S., Hsi, Y., Purswani, P., Johns, R.T., Shokouhi, P., Huang, X., and Karpyn, Z., *Frontiers in Water* (2022)

Abstract

Digital rock physics has seen significant advances owing to improvements in micro-computed tomography (MCT) imaging techniques and computing power. These advances allow for the visualization and accurate characterization of multiphase transport in porous media. Despite such advancements, image processing and particularly the task of denoising MCT images remains less explored. As such, selection of proper denoising method is a challenging optimization exercise of balancing the tradeoffs between minimizing noise and preserving original features. Despite its importance, there are no comparative studies in the geoscience domain that assess the performance of different denoising approaches, and their effect on image-based rock and fluid property estimates. Further, the application of machine learning and deep learning-based (DL) denoising models remains under-explored. In this research, we evaluate the performance of six commonly used denoising filters and compare them to five DL-based denoising protocols, namely, noise-to-clean (N2C), residual dense network (RDN), and cycle consistent generative adversarial network (CCGAN)—which require a clean reference (ground truth), as well as noise-to-noise (N2N) and noise-to-void (N2V)—which do not require a clean reference. We also propose hybrid or semi-supervised DL denoising models which only require a fraction of clean reference images. Using these models, we investigate the optimal number of high-exposure reference images that balances data acquisition cost and accurate petrophysical characterization. The performance of each denoising approach is evaluated using two sets of metrics: (1) standard denoising evaluation metrics, including peak signal-to-noise ratio (PSNR) and contrast-to-noise ratio (CNR), and (2) the resulting image-based petrophysical properties such as porosity, saturation, pore size distribution, phase connectivity, and specific surface area (SSA). Petrophysical estimates show that most traditional filters perform well when estimating bulk properties but show large errors for pore-scale properties like phase connectivity. Meanwhile, DL-based models give mixed outcomes, where supervised methods like N2C show the best performance, and an unsupervised model like N2V shows the worst performance. N2N75, which is a newly proposed semi-supervised variation of the N2N model, where 75% of the clean reference data is used for training, shows very promising outcomes for both traditional denoising performance metrics and petrophysical properties including both bulk and pore-scale measures. Lastly, N2C is found to be the most computationally efficient, while CCGAN is found to be the least, among the DL-based models considered in this study. Overall, this investigation shows that

application of sophisticated supervised and semi-supervised DL-based denoising models can significantly reduce petrophysical characterization errors introduced during the denoising step. Furthermore, with the advancement of semi-supervised DL-based models, the requirement of clean reference or ground truth images for training can be reduced and deployment of fast X-ray scanning can be made possible.

Selected Journal Publications (Last Five Years)

1. Yoga, H. F., Gasimli, N. R., and Johns, R. T., Reliable Equivalent Alkane Carbon Number Determination for Dead and Live Crudes in Microemulsion Systems, SPE Journal 29 (09), 4935-4949, 2024
2. Purswani, P., Johns, R. T., and Karpyn, Z. T., Relationship Between Residual Saturations and Wettability Using Pore-Network Modeling. *SPE J.* 29 (2024): 2004–2013.
3. Purswani, P., Johns, R. T., & Karpyn, Z. T. (2024). Impact of wettability on capillary phase trapping using pore-network modeling. Adv. Wat. Res. 184, 104606.
4. Yoga, H.F., Johns, R.T., and Prakash P., Predictive Model for Relative Permeability Using Physically Constrained Artificial Neural Networks, SPEJ 29 (02), pp. 928-942. 2024.
5. Mukherjee, S., Johns, R.T., Foroughi, S., and Blunt, M.J., Fluid-Fluid Interfacial Area and Its Impact on Relative Permeability: A Pore Network Modeling Study, SPEJ, 28(02), pp 653-663. 2023
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8. Tawfik, M. S., Karpyn, Z. T., & Johns, R. T. (2022). Effect of oil chemistry on the performance of low-salinity waterflooding in carbonates: An integrated experimental approach. Fuel, 329, [125436].
9. Mukherjee, S., & Johns, R. T. (2022). Sensitivity Analysis of Fluid–Fluid Interfacial Area, Phase Saturation and Phase Connectivity on Relative Permeability Estimation Using Machine Learning Algorithms. Energies, 15(16), [5893].
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DNA Methylation Changes Originate in Prostate Cancer Precursor Lesions

by William Nelson, Member EUAS

Short Biography

Dr. Nelson serves as the Marion I. Knott Professor and Director of the Sidney Kimmel Comprehensive Cancer Center at Johns Hopkins, and as Professor and Director of the Department of Oncology/ He is also a Professor of Medicine, Pharmacology, Pathology, Radiation Oncology, Urology, and Environmental Health Sciences. After receiving his undergraduate degree in Chemistry at Yale University, he earned doctoral degrees in Medicine and Pharmacology at the Johns Hopkins School of Medicine, and then completed Internship and Residency training in Internal Medicine and a Fellowship in Medical Oncology at the Johns Hopkins Hospital.

Dr. Nelson has directed his research efforts toward prostate cancer epigenetics, having now authored 347 articles and book chapters, attracting >42,000 citations with an h-index of 108, conducted >300 podcast interviews and provided expert opinions for >400 additional podcasts, and garnered 14 issued patents from the US Patent and Trade Office. He is most recognized for discovering the most common somatic genome alteration in human prostate cancer, a DNA methylation change affecting the GSTP1 gene, and for redirecting etiologic studies of prostatic carcinogenesis toward chronic/recurrent inflammation and the principal disease driver. He is currently a member of the Board of the V Foundation, the Scientific Chair for Stand Up 2 Cancer, and the Scientific Advisory Board for the Prostate Cancer Foundation, the Chair of the Board for Break Through Cancer, and the Executive Editor of Cancer Today.

DNA Methylation Changes Originate in Prostate Cancer Precursor Lesions

Somatic epigenetic alterations accompany the development of most human cancers, including prostate cancer (1-3). These changes, which affect chromatin structure and function, can be maintained through mitosis, providing a selective advantage for growth and survival during cancer pathogenesis. Cancer-associated epigenetic defects include: *(i)* transcriptional

silencing of caretaker genes and tumor suppressor genes, *(ii)* reactivation of embryonic genes, *(iii)* loss of imprinted gene partitioning into active and inactive alleles, *(iv)* redirection of transcription promoter use, *(v)* disordered microRNA gene expression, (vii) activation of retrotransposition, and *(viii)* increased genetic recombination at repeat elements.

The architecture of the epigenome, established in normal cells as part of development, is maintained through somatic cell mitosis as a consequence of "marks" present in genomic DNA and in chromatin proteins. The major DNA mark is symmetric methylation of cytosine bases in the self-complementary nucleotide sequence CpG. Most CpG dinucleotides carry this mark; unmethylated CpGs, clustered into ~1 kb regions encompassing the transcription start sites of many genes, have been termed "CpG islands" (4). Somatic changes in DNA methylation at CpG islands affect gene activity: genes with unmethylated CpG islands are competent for regulated transcription, responding to signaling cues by recruiting *trans*-activating factors which modify nucleosome and chromatin structure, using histone acetyltransferases (HATs) and histone methyltransferases (HMTs) to promote transcript synthesis by RNA polymerases, while genes with methylated CpG islands tend to be incompetent for expression, tightly wound around nucleosomes in a repressive chromatin structure maintained by histone deacetylases (HDACs) and other enzymes. Thus, somatic increases in CpG island methylation in cancer cells have been associated with gene silencing and heterochromatinization, while somatic decreases in DNA methylation have been implicated in illegitimate gene activation, retrotransposition, and recombination.

Changes in CpG island methylation and epigenetic gene silencing, appear to be the earliest somatic genome changes yet recognized in human prostate cancer. The most studied gene affected by *de novo* methylation during prostatic carcinogenesis is *GSTP1*, which encodes an enzyme responsible for detoxifying electrophiles and oxidants, including those that threaten cell and genome damage (5,6). Hypermethylation of *GSTP1* transcriptional regulatory sequences has been detected in more than 90% of prostate cancers in more than 50 independent analyses, far more frequently than any other known somatic gene defect (3). Loss of GSTP1 function likely occurs at the initiation of prostatic carcinogenesis, with *GSTP1* hypermethylation evident in some 5-10% of proliferative inflammatory atrophy (PIA) lesions, the earliest PCA precursors, and in more than 70% of prostatic intraepithelial neoplasia (PIN) lesions (7,8). Human prostate cancer cells devoid of GSTP1 tend to activate heterocyclic amine carcinogens, such as those found in overcooked meats, to mutagenic species (9). In addition, loss GSTP1 function also alters prostate

cancer cell responses to oxidant damage, leading to oxidation "tolerance" (10).

As of yet, the mechanism by which *GSTP1* is subjected to *de novo* methylation is not known. However, the presence of *GSTP1* hypermethylation in a subset of proliferative inflammatory atrophy (PIA) lesions, which arise in response to epithelial damage, along with the nearly ubiquitous appearance of the epigenetic defect in prostatic intraepithelial neoplasia (PIN) lesions and in prostate cancers, hints that epithelial stress might contribute to the initial steps in epigenetic gene silencing (41). Of interest, most epithelial cells in PIA and early PIN lesions express very high levels of GSTP1, likely in response to some sort of induction of *GSTP1* transcription (11,12). Rare epithelial cells in such lesions show loss of GSTP1 expression. Could the *GSTP1* transcriptional regulatory region be more vulnerable to heterochromatization when in an induced state? Certainly, if epigenetically silenced genes first arise in epithelial cells in response to stress, such as is seen in PIA and early PIN, this might comprise a recurrent theme for epithelial carcinogenesis generally, providing mechanistic insights to how epigenomes are corrupted during epithelial carcinogenesis. Intriguingly in this regard, PIA lesions with GSTP1 methylation changes tend to show intermediate levels of methylated CpG dinucleotides within the GSTP1 CpG island when compared to normal epithelium, PIN, and prostate cancer (13).

In addition to *GSTP1*, > 5000 genome sites appear to be targets of DNA hypermethylation in prostate cancers, with 73% of the regions located near genes (5', 3', or intron-exon junctions) and 27% of the regions located at conserved intergenic sites, a finding largely confirmed by ensuing studies (14,15). Whether these changes arise as part of some sort of methylation "catastrophe" in PIA or other prostate cancer precursors, or accumulate more continuously in prostate cells through neoplastic transformation and malignant cancer progression, has not been determined. What has become clear is that the somatic DNA methylation changes seen in prostate cancers are truly "drivers" of the neoplastic phenotype. Simultaneous genome-wide assessment of epigenetic and genetic alterations in lethal metastatic prostate cancers recovered at autopsy have revealed that abnormal increases (but not decreases) in DNA methylation, particularly if associated with changes in gene function, were clonally maintained throughout metastatic dissemination (16). As such, DNA hypermethylation changes appeared as subject to selection during prostate cancer pathogenesis as somatic genetic alterations.

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New Aspects in Gas Turbine Heat Transfer and Experimental Heat Transfer Methods

by Srinath Ekkad, Member EUAS

Short Biography

Srinath V. Ekkad (born 10 Nov 1968) is currently the Department Head and RJ Reynolds Professor in the Mechanical & Aerospace Engineering Department at North Carolina State University. He has made seminal contributions to the field of heat transfer as a whole, in particular to experimental heat transfer methods and also to applications in gas turbine heat transfer and cooling systems, electronic systems, and heat exchange solutions to other industrial applications over the past 25 years. He has held positions at Rolls-Royce Aircraft Engines, Louisiana State University, and Virginia Tech prior to his current appointment. He has conducted many funded projects (over $15 million) for various agencies including NSF, DARPA, DOE, Siemens, Rolls-Royce, Solar Turbines, GE among others. He has supervised 32 PhD, 50 MS students, 5 post-docs and hosted 5 visiting scholars since 1998. He has authored over 360 refereed technical publications (including 140 journal papers, 5 book chapters, and 220 refereed conference papers), 4 United States patents and one book (Gas Turbine Heat Transfer and Cooling Technology, 1st and 2nd Editions). His publications have received over 11000+ citations with a H-index of 54 according to Google Scholar.

Prof. Srinath Ekkad has been active in serving in national and international professional societies. He has served on many review panels for NSF proposals and workshop presentations for DOE advanced gas turbine research. He is a Fellow of ASME and an Associate Fellow of AIAA. He also serves on the AIAA Department Chairs/Heads committee. In the past, he has also served as Associate Member of the AIAA Thermophysics committee. He has reviewed many papers for AIAA journals and conferences in the past 20 years. He has served as session organizer or chair for more than 50 international conference technical sessions. He has also served as committee chair and conference chair for several important conferences including the Point Contact-Heat Transfer for IGTI Turbo Expo in Vienna in 2004. He handled over 35 sessions and 140 papers as Point Contact. He has also served as the coordinating scientist in the International Scientific Committee, 8th ISHMT/ASME Joint Heat and Mass Transfer Conference, Hyderabad, India, January 2008. He was the primary contact from the USA involved in inviting one plenary and six keynote speakers from US to travel to India to make presentations. He also helped organize and review papers for the US authors. In tandem with the conference, he organized an international workshop on Gas Turbine Heat Transfer Workshop at IIT-Madras in January 2008. Attended by 40 gas turbine engineers and researchers from various organizations in India. Four US and three Indian Researchers presented to the audience with ensuing discussions. One of his major contributions has been as the Technical Chair for the Summer Heat Transfer Conference, held in Minneapolis, July 2013, which coincided with the 75th Anniversary of ASME Heat Transfer Division, attended by over 800 heat transfer researchers. He currently serves on the ASME Mechanical Engineering Department Heads Executive Committee. He has been invited for more than 30 seminars including a few keynotes at various national and international conferences (India, China, Europe). He was recently invited to serve on a panel of experts on the future of gas turbine and propulsion technology by Government of India which will be held on October 9, 2020. He also serves on Advisory Board for National Institute for Aerospace (NIA)

He was the inaugural recipient of the ASME Bergles/Rohsenow Young Investigator in Heat Transfer in 2004 for significant contributions to the field of heat transfer by a researcher under the age of 36. Since then he has received the Virginia Tech Dean of Engineering Research Excellence Award in 2012 and the Virginia Tech Alumni Association for Excellence in Graduate Advising

Award in 2014. He also received the Rolls-Royce Commonwealth Endowed Professorship from Virginia Tech in 2012 and the RJ Reynolds Professor from NC State University in 2017. He has served as Associate Editor for three major heat transfer journals and in July 2019, he was chosen to be the new Editor-in-Chief for the ASME Journal for Thermal Science and Engineering Applications, one of the flagship journals for the ASME Heat Transfer Division. In June 2019, he was awarded outstanding service award for the ASME IGTI committee on Gas Turbine Heat Transfer. He continues to serve on the committee. Dr. Ekkad has also served as a summer faculty fellow at AFRL, Dayton in 2003. He is also the Editor-in-Chief for the ASME Journal for Thermal Science and Engineering Applications. He received the 2022 AIAA Air Breathing Propulsion Award and the 2022 ASME Heat Transfer Memorial Award and was named a fellow of the Royal Aeronautical Society in 2023 and Fellow of AIAA in 2024.

His original contributions can be summarized as follows:

Textbook on Gas Turbine Heat Transfer

Professor Ekkad has developed a large body of fundamental knowledge that formed the basis of a comprehensive textbook on heat transfer in turbomachinery (JC Han, S Dutta, S Ekkad, Gas Turbine Heat Transfer and Cooling Technology, CRC press, 2012.). This book has been adopted widely as a graduate-level textbook as well as a research resource, becoming the definitive source of fundamental educational and reference materials on this field of heat transfer application, which is one of the pillars of technological progress that our discipline has produced in its rich history.

New Textbook on Experimental Heat Transfer Methods

Professor Ekkad is currently working on a new book that focuses on design and development of experimental heat transfer methods using fundamental and applied knowledge of heat transfer phenomena and also optical technology. The book will focus on providing historical methods and also provide very detailed background on new methods focused on detailed measurements. This book will be published by Cambridge University Press in 2021.

Invited Review Papers

Professor Ekkad was invited to submit two review papers on his work. The first review paper is published on “Novel Jet Impingement Heat Transfer Methods - A Modern Review” in ASME Journal of Heat Transfer. The paper has been accepted and will be published soon. This paper presents an update on novel impingement cooling methods that have been developed to enhance heat transfer effectiveness of impinging jets. The second paper published on “Detailed Heat Transfer Measurements for Rotating Turbulent Flows in Gas Turbine Systems,” is in the Journal Energies. This paper provides an overview of novel measurement methods used by researchers to make very highly detailed heat transfer measurements in rotating channels.

Transient Heat Transfer Measurement Methods

In the early 1990s, Professor Ekkad learned the transient liquid crystal measurement technique for detailed 2-D surface heat transfer measurements as a MS student at Arizona State University under Dr. Darryl Metzger (late). During his PhD with Prof. Han at Texas A&M University, Prof. Ekkad further developed the technique and provided considerable visibility to the method of evaluation and improved uncertainty and utility. During this time, Prof. Ekkad implemented this technique to study very complex geometries like rib turbulated

channels (Ekkad and Han, IJHMT, 40, 2525, 1997); Compound angle film cooling (Ekkad et al., ASME J. Turbomachinery, 119, 587, 1997); Leading edge film cooling (Ekkad et al., ASME J. Turbomachinery, 119, 580, 1997); Turbine airfoil cooling (Du et al., ASME J. Turbomachinery 120, 808, 1997) in addition to jet impingement cooling (Huang et al., ASME J. Turbomachinery, 12, 73, 1998). The 1997 IJHMT paper on rib turbulated channels was the first paper to present detailed heat transfer coefficient measurements inside such channels. Prof. Ekkad's major contributions at Texas A&M developing the liquid crystal technique are summarized in the paper by Ekkad and Han (Measurement Science and Technology 11, 957, 2000). In 2003, Professor Ekkad developed a similar measurement technique using Infrared Thermography while he was at AFRL. The work was presented in a paper by Ekkad et al. (ASME J. Turbomachinery, 126, 597, 2004). Professor Ekkad then implemented this technique for other gas turbine geometries including turbine blade tip heat transfer and cooling (Nasir et al., ASME J. Turbomachinery 126, 221, 2004). Recently, Professor Ekkad has implemented the transient liquid crystal technique for detailed heat transfer measurements inside rotating turbine blade cooling channels. Today, the impact of all the liquid crystal work is indicated by the number of papers using the transient liquid crystal technique that have been published. The technique is now considered a standard method to measure heat transfer coefficients for complex flow geometries.

Gas Turbine Combustor Heat Transfer

In the early 2000s, Professor Ekkad was the first to propose studying convective heat load on gas turbine combustor liner walls. He was one of the first to publish in open literature on this important problem and developed the topic to be a stand-alone topic at the annual Turbo Expo held by ASME IGTI. Today, the conference hosts 3-4 sessions with over 15 papers in the topic. One of the first papers by Professor Ekkad on this topic was at the Turbo Expo in 2008 and the paper is now in the ASME archive (Patil et al., ASME J. Turbomachinery, 133, 011028, 2011). Since then Professor Ekkad has published ten journal papers on the topic and is now studying combustor liner heat transfer under reacting flow conditions, which has never been studied in open literature. Professor Ekkad has also published papers on combustor liner backside cooling with a seminal paper by Esposito et al. (ASME JTSEA, 1, 021001, 2009).

Film Cooling Geometries and Jet Impingement

Professor Ekkad has developed innovative cooling hole geometries over the past 20 years. He has published papers in 2006 and 2007 on novel hole shapes with Yiping Lu, his PhD student. In 2007, he also presented a novel anti-vortex or tripod hole that was published in two pioneering papers (Heidmann and Ekkad, ASME J. Turbomachinery, 130, 031020, 2008; Dhungel et al., ASME J. Turbomachinery, 131, 021007, 2009). This film hole provides much better cooling coverage using half the amount of cooling air compared to traditional film holes used in current gas turbine blades. In 2007, Professor Ekkad also studied unique film holes that are embedded in trenches or craters to reduce mixing and improve coolant coverage. Two other papers (Lu et al., ASME J. Turbomachinery, 131, 011003 & 011005, 2009) were also significantly impactful with over fifty papers published on this topic after these two papers. Improved film cooling with reduced coolant flow usage is now the focus of many studies and the efforts in new film hole shapes in the form of sister holes, exit shapes, and diffused holes are the results of the impact of Dr. Ekkad's work.

Impingement cooling is one of the most efficient heat transfer technique employed in many practical problems. Professor Ekkad has made extensive contributions in the area of

improved jet impingement cooling. Prof. Ekkad studied the combined of swirl and impingement when he was at LSU (e.g., Pamula et al., ASME J. Turbomachinery, 123, 281, 2001). Other than significant papers in the 1990s and 2000s, Prof. Ekkad has made impingement cooling design studies for power systems module cooling (e.g., Parida et al., International Journal of Thermal Sciences 50, 1037, 2011). The novel impingement cooling designs were used to cool the control power unit for a hybrid electric vehicle. Prof. Ekkad has also investigated impingement cooling in the presence of metal foams in his recent work published by ASME (Madhavan et al., ASME JTSEA, 11, 061016, 2019). He has also investigated swirl cooling through impingement holes with a to-be published paper at the IMECE using impingement holes that have screw grooves. These innovative jet impingement studies have furthered the effectiveness of impingement cooling/heating designs for a variety of applications including electronic cooling, gas turbine cooling, and automotive systems.

Rotational Effects on Channel Heat Transfer

Making detailed heat transfer measurements inside rotating channels is a challenging problem. Professor Ekkad has been making detailed heat transfer measurements in rotating channels for the past decade or so. He developed a unique methodology to measure detailed heat transfer distributions under rotation in 2010 using liquid crystals and a transient experiment. Recent work (e.g., Singh et al., International Journal of Heat and Mass Transfer 132, 80-95, 2019) captures the effect of rotation inside complex channels with turns and rib turbulators and impingement jets. This kind of detailed measurements inside rotating channels had never been achieved before Prof. Ekkad's contributions. This is a relatively new area and has already shows that Dr. Ekkad continues to innovate with new experimental methods to solve complex heat transfer problems.

PUBLICATIONS:

Book

1. JC Han, S Dutta, S Ekkad, *Gas Turbine Heat Transfer and Cooling Technology*, CRC press, 2012.
   This book has become the de facto standard of rigor and practice in the field. It has been cited over 2200 times.

Transient Heat Transfer Measurement Methods

2. SV Ekkad, JC Han, "Detailed heat transfer distributions in two-pass square channels with rib turbulators," International Journal of Heat and Mass Transfer 40 (11), 2525-2537, 1997.
   The first paper to provide detailed heat transfer measurements inside ribbed channels and has been cited nearly 400 times.
3. SV Ekkad, D Zapata, JC Han, "Film effectiveness over a flat surface with air and CO2 injection through compound angle holes using a transient liquid crystal image method," ASME Journal of Turbomachinery 119 (3), 587-593, 1997 (Cited 207 times)
4. SV Ekkad, S Ou, RB Rivir, "A transient infrared thermography method for simultaneous film cooling effectiveness and heat transfer coefficient measurements from a single test," ASME Journal of Turbomachinery 126 (4), 597-603, 2004. (Cited 173 times)
   This work represents the first comprehensive use of infrared thermography to quantify unsteady cooling of turbomachinery and has since become widely adopted in practice.
5. H Nasir, SV Ekkad, DM Kontrovitz, RS Bunker, C Prakash, "Effect of tip gap and squealer geometry on detailed heat transfer measurements over a high pressure turbine rotor blade tip," ASME Journal of Turbomachinery 126 (2), 221-228, 2004. (*used Infrared Technique)*
6. SV Ekkad, JC Han, "A transient liquid crystal thermography technique for gas turbine heat transfer measurements," Measurement Science and Technology 11 (7), 957, 2000.

This work was detailed review of the implementation of the transient liquid crystal technique for complex geometries that exist in gas turbine systems. (Cited 254 times)

Gas Turbine Combustor Heat Transfer

7. S Patil, S Abraham, D Tafti, S Ekkad, Y Kim, P Dutta, HK Moon, R. Srinavasan, "Experimental and numerical investigation of convective heat transfer in a gas turbine can combustor," ASME Journal of Turbomachinery 133 (1), 011028, 2011. (Cited 58 times)

   This paper, first published in conference form in 2008, formed the basis of a new branch of study, leading to regular multi-session conference presentations from the community.

8. EI Esposito, SV Ekkad, Y Kim, P Dutta, "Novel jet impingement cooling geometry for combustor liner backside cooling," ASME Journal of Thermal Science and Engineering Applications 1 (2), 021001, 2009. (Cited 72 times)

Film Cooling Geometries

9. JD Heidmann, S Ekkad, "A novel antivortex turbine film-cooling hole concept," ASME Journal of Turbomachinery, 130 (3), 031020, 2008. (Cited 179 times)
10. A Dhungel, Y Lu, W Phillips, SV Ekkad, J Heidmann, "Film cooling from a row of holes supplemented with antivortex holes," ASME Journal of Turbomachinery 131 (2), 021007, 2009. (Cited 114 times)

    Papers 9 and 10, in combination, presented a new method to shape cooling holes for improved heat transfer performance, and the approach has formed the basis of a large body of related work by the community.

11. Y Lu, A Dhungel, SV Ekkad, RS Bunker, "Effect of trench width and depth on film cooling from cylindrical holes embedded in trenches," ASME Journal of Turbomachinery 131 (1), 011003, 2009. (Cited 56 times)

Advanced Jet Impingement Cooling

12. S Madhavan, P Singh, S Ekkad, "Jet Impingement Heat Transfer Enhancement by Packing High-Porosity Thin Metal Foams Between Jet Exit Plane and Target Surface," Journal of Thermal Science and Engineering Applications 11 (6), 061016, 2019.
13. Ekkad, S. V., and Singh, P. (January 5, 2021). "A Modern Review on Jet Impingement Heat Transfer Methods." ASME. J. Heat Transfer. *This is the latest paper that highlights all our novel jet impingement work in the past decade.*

Rotational Effects on Channel Heat Transfer

14. Singh, P., Li, W., Ekkad, S.V., Ren, J., 2017, "Experimental and numerical investigation of heat transfer inside two-pass rib roughened duct (AR=1:2) under rotating and stationary conditions", Int. J. Heat Mass Transfer, Vol. 113, pp. 384-398, *This work was one of the first papers to demonstrate the viability of transient liquid crystal technique for rotating channels.*
15. Ekkad, S.V.; Singh, P. Detailed Heat Transfer Measurements for Rotating Turbulent Flows in Gas Turbine Systems. Energies 2021, 14, 39. *This paper provides much detail into all our detailed measurement work into rotating channels.*

PATENTS:

1. A Transient Infrared Thermography Method for Simultaneous Film Cooling Effectiveness and Heat Transfer Measurements from a Single Test, Ou, S., Ekkad, S. V., and Rivir, R. B, US patent # 7,040,805.
2. Zero Cross Flow Impingement through an Array of Extended Ports, Ekkad, S.V., Kim, Y. W., and Esposito, E., US Patent # 8,127,553.
3. A Combination Cooling Method involving Swirl, Impingement and Plate Fins, Ekkad, S.V., and Parida, P., Disclosure.
4. Transpiration Cooling of Turbine Airfoils using ODS Architectures, Alvin, M.A., Anderson, I., Heidloff, A., Miller, N., Siew, S.C., Reddy, B.K.V., Chyu, M.K., Klinger, J., Paulus, J., McMordie, B., Ekkad, S.V., Ramesh, S., disclosure submitted through DOE-NETL.

Shiga Toxin-Producing Escherichia Coli and the Hemolytic-Uremic Syndrome

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 2018 Professor Remuzzi has also taken on the role of Director of the Mario Negri Institute. He has been member of the Consiglio Superiore di Sanità since February 2019. He has been Vice President of the Italian Institute for Planetary Health since 2019.

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 awarded the "Lennox K. Black International Prize for Excellence in Medicine" at the Thomas Jefferson University in Philadelphia.

In 2022 he was honoured by the Italian President of the Republic with the title of Cavaliere di Gran Croce.

Prof. Remuzzi is the author of hundreds of publications in International medical journals and has written 24 books. He also regularly writes editorials for the Corriere della Sera newspaper.

N Engl J Med. 2023 Dec 28;389(26):2499

Shiga Toxin-Producing Escherichia coli and the Hemolytic-Uremic Syndrome

Marina Noris, Giuseppe Remuzzi

Abstract

In their review, Freedman et al. (Oct. 12 issue) dedicate only a few lines to complement activation. However, several studies have shown that complement plays an important role in the pathophysiology of Shiga toxin–producing *Escherichia coli* (STEC)–associated hemolytic–uremic syndrome (HUS). Shiga toxins have been shown to induce C3b deposition on human cultured endothelial cells. In human whole blood, Shiga toxin 2 promoted the formation of C3- and C5b-9–coated red cell–derived microvesicles. Glomerular C3 and C5b-9 deposits have been found in mice and children with STEC-associated HUS. Deficiency of the key component of the complement alternative pathway factor B protected mice from Shiga toxin 2–induced renal dysfunction. Low C3 levels and elevated plasma levels of breakdown products of C3 and factor B were found in patients with STEC-associated HUS and were predictive of severe complications. Finally, despite the fact that complement gene mutations are rare, the authors' statement that pathogenic gene variants "are not associated with the severity of illness" does not seem correct. In fact, cases involving patients with severe STEC-associated HUS and complement gene mutations have been described, and complement inhibition with the use of eculizumab was lifesaving in those children.

BMJ. 2023 May 31:381:e073654.

Race-free estimated glomerular filtration rate equation in kidney transplant recipients: development and validation study

Marc Raynaud, Solaf Al-Awadhi, Ivana Juric, Gillian Divard, Yannis Lombardi, Nikolina Basic-Jukic, Olivier Aubert, Laurence Dubourg, Ingrid Masson, Christophe Mariat, Dominique Prié, Vincent Pernin, Moglie Le Quintrec, Timothy S Larson, Mark D Stegall, Boris Bikbov, Piero Ruggenenti Laurent Mesnard, Hassan N Ibrahim, Marie Bodilsen Nielsen, Arthur J Matas, Brian J Nankivell, Stan Benjamens, Robert A Pol, Stephan J L Bakker, Xavier Jouven, Christophe Legendre, Nassim Kamar, Byron H Smith, Hani M Wadei, Antoine Durrbach, Flavio Vincenti, Giuseppe Remuzzi, Carmen Lefaucheur, Andrew J Bentall, Alexandre Loupy

Abstract

Objective: To compare the performance of a newly developed race-free kidney recipient specific glomerular filtration rate (GFR) equation with the three current main equations for measuring GFR in kidney transplant recipients.
Design: Development and validation study SETTING: 17 cohorts in Europe, the United States, and Australia (14 transplant centres, three clinical trials).
Participants: 15 489 adults (3622 in development cohort (Necker, Saint Louis, and Toulouse hospitals, France), 11 867 in multiple external validation cohorts) who received kidney transplants between 1 January 2000 and 1 January 2021.
Main outcome measure: The main outcome measure was GFR, measured according to local practice. Performance of the GFR equations was assessed using P30 (proportion of estimated GFR (eGFR) within 30% of measured GFR (mGFR)) and correct classification (agreement between eGFR and mGFR according to GFR stages). The race-free equation, based on creatinine level, age, and sex, was developed using additive and multiplicative linear regressions, and its performance was compared with the three current main GFR equations: Modification of Diet in Renal Disease (MDRD) equation, Chronic Kidney Disease Epidemiology Collaboration (CKD-EPI) 2009 equation, and race-free CKD-EPI 2021 equation.
Results: The study included 15 489 participants, with 50 464 mGFR and eGFR values. The mean GFR was 53.18 mL/min/1.73m2 (SD 17.23) in the development cohort and 55.90 mL/min/1.73m2 (19.69) in the external validation cohorts. Among the current GFR equations, the race-free CKD-EPI 2021 equation showed the lowest performance compared with the MDRD and CKD-EPI 2009 equations. When race was included in the kidney recipient specific GFR equation, performance did not increase. The race-free kidney recipient specific GFR equation showed significantly improved performance compared with the race-free CKD-EPI 2021 equation and performed well in the external validation cohorts (P30 ranging from 73.0% to 91.3%). The race-free kidney recipient specific GFR equation performed well in several subpopulations of kidney transplant recipients stratified by race (P30 73.0-91.3%), sex (72.7-91.4%), age (70.3-92.0%), body mass index (64.5-100%), donor type (58.5-92.9%), donor age (68.3-94.3%), treatment (78.5-85.2%), creatinine level (72.8-91.3%), GFR measurement method (73.0-91.3%), and timing of GFR measurement post-transplant (72.9-95.5%). An online application was developed that estimates GFR based on recipient's creatinine level, age, and sex
Conclusion: A new race-free kidney recipient specific GFR equation was developed and validated using multiple, large, international cohorts of kidney transplant recipients. The equation showed high accuracy and outperformed the race-free CKD-EPI 2021 equation that was developed in individuals with native kidneys.

Lancet Infect Dis. 2023 Jan;23(1):e22-e33.

Home as the new frontier for the treatment of COVID-19: the case for anti-inflammatory agents

Norberto Perico, Monica Cortinovis, Fredy Suter, Giuseppe Remuzzi

Abstract

COVID-19, caused by SARS-CoV-2, is characterised by a broad spectrum of symptom severity that requires varying amounts of care according to the different stages of the disease. Intervening at the onset of mild to moderate COVID-19 symptoms in the outpatient setting would provide the opportunity to prevent progression to a more severe illness and long-term complications. As early disease symptoms variably reflect an underlying excessive inflammatory response to the viral infection, the use of anti-inflammatory drugs, especially non-steroidal anti-inflammatory drugs (NSAIDs), in the initial outpatient stage of COVID-19 seems to be a valuable therapeutic strategy. A few observational studies have tested NSAIDs (especially relatively selective COX-2 inhibitors), often as part of multipharmacological protocols, for early outpatient treatment of COVID-19. The findings from these studies are promising and point to a crucial role of NSAIDs for the at-home management of people with initial COVID-19 symptoms.

J Am Soc Nephrol. 2023 Oct 1;34(10):1733-1751.

Safety and Preliminary Efficacy of Mesenchymal Stromal Cell (ORBCEL-M) Therapy in Diabetic Kidney Disease: A Randomized Clinical Trial (NEPHSTROM)

Norberto Perico, Giuseppe Remuzzi, Matthew D Griffin, Paul Cockwell, Alexander P Maxwell, Federica Casiraghi, Nadia Rubis, Tobia Peracchi, Alessandro Villa, Marta Todeschini, Fabiola Carrara, Bernadette A Magee, Piero L Ruggenenti, Stefano Rota, Laura Cappelletti, Veronica McInerney, Tomás P Griffin, Md Nahidul Islam, Martino Introna, Olga Pedrini, Josée Golay, Andrew A Finnerty, Jon Smythe, Willem E Fibbe, Stephen J Elliman, Timothy O'Brien.

Abstract

Significance statement: Mesenchymal stromal cells (MSCs) may offer a novel therapy for diabetic kidney disease (DKD), although clinical translation of this approach has been limited. The authors present findings from the first, lowest dose cohort of 16 adults with type 2 diabetes and progressive DKD participating in a randomized, placebo-controlled, dose-escalation phase 1b/2a trial of next-generation bone marrow-derived, anti-CD362 antibody-selected allogeneic MSCs (ORBCEL-M). A single intravenous (iv) infusion of 80×10 6 cells was safe and well-tolerated, with one quickly resolved infusion reaction in the placebo group and no subsequent treatment-related serious adverse events (SAEs). Compared with

placebo, the median annual rate of decline in eGFR was significantly lower with ORBCEL-M, although mGFR did not differ. The results support further investigation of ORBCEL-M in this patient population in an appropriately sized phase 2b study.

Background: Systemic therapy with mesenchymal stromal cells may target maladaptive processes involved in diabetic kidney disease progression. However, clinical translation of this approach has been limited.

Methods: The Novel Stromal Cell Therapy for Diabetic Kidney Disease (NEPHSTROM) study, a randomized, placebo-controlled phase 1b/2a trial, assesses safety, tolerability, and preliminary efficacy of next-generation bone marrow-derived, anti-CD362-selected, allogeneic mesenchymal stromal cells (ORBCEL-M) in adults with type 2 diabetes and progressive diabetic kidney disease. This first, lowest dose cohort of 16 participants at three European sites was randomized (3:1) to receive intravenous infusion of ORBCEL-M (80×10 6 cells, n =12) or placebo (n =4) and was followed for 18 months.

Results: At baseline, all participants were negative for anti-HLA antibodies and the measured GFR (mGFR) and estimated GFR were comparable between groups. The intervention was safe and well-tolerated. One placebo-treated participant had a quickly resolved infusion reaction (bronchospasm), with no subsequent treatment-related serious adverse events. Two ORBCEL-M recipients died during follow-up of causes deemed unrelated to the trial intervention; one recipient developed low-level anti-HLA antibodies. The median annual rate of kidney function decline after ORBCEL-M therapy compared with placebo did not differ by mGFR, but was significantly lower by eGFR estimated by the Chronic Kidney Disease Epidemiology Collaboration and Modification of Diet in Renal Disease equations. Immunologic profiling provided evidence of preservation of circulating regulatory T cells, lower natural killer T cells, and stabilization of inflammatory monocyte subsets in those receiving the cell therapy compared with placebo.

Conclusions: Findings indicate safety and tolerability of intravenous ORBCEL-M cell therapy in the trial's lowest dose cohort. The rate of decline in eGFR (but not mGFR) over 18 months was significantly lower among those receiving cell therapy compared with placebo. Further studies will be needed to determine the therapy's effect on CKD progression.

Am J Kidney Dis. 2024 May;83(5):588-600.e1.

Anti-Phospholipase A2 Receptor 1 and Anti-Cysteine Rich Antibodies, Domain Recognition and Rituximab Efficacy in Membranous Nephropathy: A Prospective Cohort Study

Piero Ruggenenti , Linda Reinhard, Barbara Ruggiero, Annalisa Perna, Luca Perico, Tobia Peracchi, Diego Fidone, Alessia Gennarini, Ariela Benigni, Monica Cortinovis, Elion Hoxha, Giuseppe Remuzzi

Abstract

Rationale & objective: Proteinuria and anti-phospholipase A_2 receptor 1 (anti-PLA_2R1) antibody titers are associated with primary membranous nephropathy (MN) outcomes. We evaluated the association of antibodies against the cysteine-rich (CysR) and C-type lectin 1, 7, and 8 (CTLD1, CTLD7, and CTLD8) domains of PLA_2R1 with MN outcomes.
Study design: Prospective cohort study.
Setting & participants: One-hundred-thirteen consecutive, consenting patients referred to the Nephology Unit of the Azienda-Socio-Sanitaria-Territoriale (ASST) Papa Giovanni XXIII (Bergamo, Italy) with PLA_2R1-related, biopsy-proven MN whose persistent nephrotic syndrome (NS) was managed conservatively for>6 months and were monitored with serial evaluations of proteinuria, autoantibodies (by enzyme-linked immunosorbent assay), and clinical outcomes.
Exposure: Rituximab.
Outcome: Complete (proteinuria<0.3g/24h) or partial (proteinuria≥0.3g/24h and<3.0g/24h with>50% reduction vs basal) NS remission.
Analytical approach: Univariable and multivariable Cox regression analyses.
Results: All patients had anti-CysR antibodies; 62 (54.9%) were multidomain recognizers. Anti-PLA_2R1 and anti-CysR antibody titers were strongly correlated at baseline (P<0.001, r=0.934), 6 months (P<0.001, r=0.964), and 12 months (P<0.001, r=0.944). During a median follow-up of 37.1 (IQR, 20.3-56.9) months, 71 patients (62.8%) achieved either complete or partial remission of their NS. Lower baseline anti-PLA_2R1 (HR, 0.997 [95% CI, 0.996-0.999], P=0.002) and anti-CysR [HR, 0.996 [95% CI, 0.993-0.998], P=0.001) titers were associated with a higher probability of remission, along with female sex, lower proteinuria, and lower serum creatinine levels (P<0.05 for all comparisons). Anti-CTLD antibodies were not associated with outcomes. At 6 and 12 months, compared to baseline, anti-PLA_2R1 and anti-CysR antibody titers decreased more in patients progressing to partial or complete remission than in those without remission (P<0.05 for all comparisons).
Limitations: Observational design.
Conclusions: In PLA_2R1-related MN, anti-PLA_2R1 and anti-CysR antibodies similarly predict rituximab efficacy independent of PLA_2R1 domain recognition. The choice between these tests should be dictated by feasibility and costs. Evaluating anti-CTLD antibodies appears unnecessary.
Plain-language summary: Primary membranous nephropathy (MN), a leading cause of nephrotic syndrome (NS) in adults, is an autoimmune disease caused by autoantibodies binding to the podocyte antigen phospholipase A2 receptor 1 (PLA_2R1). We assessed whether the effects of anti-CD20 cytolytic therapy with the monoclonal antibody rituximab are associated with detection rates and levels of anti-PLA_2R1 antibodies and antibodies against PLA_2R1 domains such as cysteine-rich (CysR), and C-type lectin 1, 7, and 8 (CTLD1, 7, and 8), in patients with PLA_2R1-related MN and persistent NS. The probability of rituximab-induced complete or partial NS remission was associated with baseline anti-PLA_2R1 and

anti-CysR antibody titers, but not with anti-CTLD1, 7 and 8 antibodies or multidomain recognition. Integrated evaluation of anti-PLA_2R1 or anti-CysR antibodies with proteinuria and kidney function may play a role in monitoring the effects of rituximab in patients with PLA_2R1-related NS and MN.
Keywords: CysR; PLA(2)R1; domain recognition; membranous nephropathy; nephrotic syndrome; rituximab; sex.

Am J Kidney Dis. 2024 Mar;83(3):340-349.e1.

Ofatumumab in Rituximab-Resistant and Rituximab-Intolerant Patients With Primary Membranous Nephropathy: A Case Series

Manuel Alfredo Podestà , Matias Trillini, Valentina Portalupi, Alessia Gennarini, Federica Tomatis, Alessandro Villa, Annalisa Perna, Nadia Rubis, Giuseppe Remuzzi, Piero Ruggenenti

Abstract

Rationale & objective: Rituximab is the first-choice therapy for patients with primary membranous nephropathy (MN) and nephrotic syndrome. However, approximately 30% of patients are treatment-resistant or become treatment-intolerant with hypersensitivity reactions upon repeated drug exposures. We aimed to assess whether ofatumumab, a fully human second-generation anti-CD20 antibody, could be a valuable alternative to rituximab in this population.
Study design: Case series.
Setting & participants: 7 rituximab-intolerant and 10 rituximab-resistant patients with MN who consented to receive ofatumumab (50-300mg, single intravenous infusion) and were followed at the nephrology unit of Azienda Socio-Sanitaria Territoriale Papa Giovanni XXIII (Bergamo, Italy) between September 2015 and January 2019.
Findings: Over a median (IQR) follow-up of 5.0 (3.0-9.8) months, all 7 rituximab-intolerant and 3 of the 10 rituximab-resistant patients exhibited complete (proteinuria<0.3g/d) or partial (proteinuria<3.5g/d with≥50% reduction vs baseline) remission of nephrotic syndrome. Circulating B cells were similarly depleted in all patients by 1 week, and serum anti-phospholipase A_2 receptor antibody concentrations decreased to<2.7 relative units/mL in 3 of 4 rituximab-intolerant and 4 of 8 rituximab-resistant patients with phospholipase A_2 receptor-related disease. Ofatumumab significantly reduced 24-hour urinary protein and immunoglobulin G excretion and increased serum albumin and immunoglobulin G levels. These effects were greater in rituximab-intolerant than in rituximab-resistant patients. Measured glomerular filtration rate significantly increased by an average of 13.4% at 24 months compared with baseline (P=0.036) among all patients in the series. There were 14 nonserious infusion-related adverse events in 9 patients that recovered with temporary infusion interruption.

Limitations: Retrospective design, limited number of patients.
Conclusions: Ofatumumab may represent an effective and safe treatment for rituximab-intolerant cases of MN. Larger prospective studies will be needed to validate these preliminary findings and explore the effectiveness of other second-generation anti-CD20 antibodies in this clinical setting.
Plain-language summary: Primary membranous nephropathy (MN) is one of the most frequent causes of nephrotic syndrome (NS) in adults. In this case series, we explored the efficacy of ofatumumab, a fully human second-generation anti-CD20 antibody, in 17 patients with MN and NS who were intolerant or unresponsive to rituximab. All 7 rituximab-intolerant patients exhibited complete or partial clinical remission, compared with only 3 of the 10 rituximab-resistant patients. Autoantibody levels decreased in all patients with phospholipase A_2 receptor-related disease. Ofatumumab achieved a significant reduction in urinary protein and immunoglobulin G excretion while increasing serum albumin and immunoglobulin G levels. Ofatumumab may be a promising option for patients with MN who are rituximab-intolerant. Further investigations are warranted to validate these preliminary findings.
Keywords: B cells; Rituximab; membranous nephropathy; nephrotic syndrome; ofatumumab.

Clin J Am Soc Nephrol. 2024 Jun 3;19(9):1201-1208.

Developing Therapies for C3 Glomerulopathy: Report of the Kidney Health Initiative C3 Glomerulopathy Trial Endpoints Work Group

Carla Nester, Dima A Decker, Matthias Meier, Shakil Aslam, Andrew S Bomback, Fernando Caravaca-Fontán, Terence H Cook, David L Feldman, Veronique Fremeaux-Bacchi, Daniel P Gale, Ann Gooch, Sally Johnson, Christoph Licht, Mohit Mathur, Matthew C Pickering, Manuel Praga, Giuseppe Remuzzi, Viknesh Selvarajah, Richard J Smith, Hossein Tabriziani, Nicole van de Kar, Yaqin Wang, Edwin Wong, Kirtida Mistry, Mark Lim, Cesia Portillo, Seyi Balogun, Howard Trachtman, Aliza Thompson

Abstract

Randomized clinical trials are underway to evaluate the efficacy of novel agents targeting the alternative complement pathway in patients with C3 glomerulopathy (C3G), a rare glomerular disease. The Kidney Health Initiative convened a panel of experts in C3G to (1) assess the data supporting the use of the prespecified trial end points as measures of clinical benefit and (2) opine on efficacy findings they would consider compelling as treatment(s) of C3G in native kidneys. Two subpanels of the C3G Trial Endpoints Work Group reviewed the available evidence and uncertainties for the association between the three prespecified end points-(1) proteinuria, (2) eGFR, and (3) histopathology-and anticipated outcomes. The full

work group provided feedback on the summaries provided by the subpanels and on what potential treatment effects on the proposed end points they would consider compelling to support evidence of an investigational product's effectiveness for treating C3G. Members of the full work group agreed with the characterization of the data, evidence, and uncertainties, supporting the end points. Given the limitations of the available data, the work group was unable to define a minimum threshold for change in any of the end points that might be considered clinically meaningful. The work group concluded that a favorable treatment effect on all three end points would provide convincing evidence of efficacy in the setting of a therapy that targeted the complement pathway. A therapy might be considered effective in the absence of complete alignment in all three end points if there was meaningful lowering of proteinuria and stabilization or improvement in eGFR. The panel unanimously supported efforts to foster data sharing between academic and industry partners to address the gaps in the current knowledge identified by the review of the end points in the aforementioned trials.

Progress on Structural Safety and Control

by Hong-Nan Li, Member EUAS

Short Biography

Dr. Hong-Nan Li received his bachelor, master and PhD degrees from China in 1982, 1987 and 1990, respectively. He had conducted his postdoctoral research at Virginia Polytechnic Institute and State University from 1992-1994 in Virginia, USA. He has been a Distinguished Professor of School of Civil Engineering at Dalian University of Technology (DUT), China since Sept. 2001. 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 for civil infrastructures. He is the author/co-author of 9 books and more than 400 refereed journal papers including more than 300 international journals. He is also an inventor or co-inventor of 83 invention patents. He has delivered over 90 keynote and invited lecture at international conferences and universities in different countries.

He ever edited the first 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: 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), etc.

Dr. Li promoted the education of undergraduate students and graduate students in Civil Engineering. He has supervised more than 60 Ph.D. students and 70 Master students. Some thesis from his students were awarded for the provincial excellent theses.

New Progress on Research Activities

1. Theoretical Solution of the Maximum Jump Height for Multi-Span Transmission Lines after Ice Shedding

Maximum jump height evaluation is crucial for transmission line deicing and typically involves time-consuming processes such as dynamic numerical simulations and model experiments. Previous studies have explored the feasibility of theoretical solutions to improve computational efficiency and proposed various simplifying assumptions during derivation to address the strong geometric nonlinearity of cable structures. However, these assumptions neglect certain measurable influencing factors, such as temperature fluctuations, tension variations between adjacent conductors, and combinations of unequal span lengths and elevation differences, hindering the applicability of existing methods. To overcome this challenge, this paper proposes a novel theoretical method to calculate the maximum jump height for multi-span transmission lines after ice shedding. The three conventionally overlooked factors are considered in derivation. The dynamic response of transmission lines is divided into two stages, i.e., the kinetic energy increases first and subsequently decreases. Then, the proposed method is validated through numerical simulations, considering span lengths, ice thicknesses, temperatures, conductor types, elevation differences, and span combinations. In addition, an ice-shedding experiment is conducted for further validation, followed by a comparison with other multiple experiments. The results demonstrate the validity and efficiency of our method, indicating a noticeable reduction in modeling and computational costs, proving its extensive potential in engineering.

2. Nataf-Based Probabilistic Multi-Dimensional Buffeting Analysis of Overhead Transmission Lines

The overhead transmission line (OTL) is a complex nonlinear mechanical system susceptible to wind load, whose buffeting seriously affects the safety of transmission towers. Conventional one-dimensional buffeting analysis overlooks potential vertical turbulence, only considering the excitation of longitudinal turbulence. Additionally, the turbulence parameters associated with the refined simulation of real stochastic wind fields are simply assumed to be deterministic. Such oversimplified schemes might result in severe misestimation of extreme responses. Hence, this paper presents a novel framework for probabilistically estimating the multi-dimensional buffeting responses of OTL. First, a two-dimensional influence line method is introduced to replace the time-consuming nonlinear finite element analysis (NFEA). After that, the Nataf transformation is

used to generate turbulence parameter samples, effectively preserving both the marginal probability distribution function (PDF) and correlation structure. Subsequently, the three-dimensional wind speed sequences are simultaneously synthesized, and the impact of turbulence parameter uncertainty on wind field characteristics is systematically investigated. Then, the buffeting responses in both time and frequency domains are analytically estimated, and a quantile-based design method is proposed by establishing the PDF of extreme responses. Finally, the tornado diagram-based sensitivity analysis is conducted to quantify the relative sensitivity of different responses to each turbulence parameter. The results show that the two-dimensional influence line algorithm exhibits significant efficiency advantages, while the NFEA approach struggles to accomplish the same task on short notice. All deterministic extreme responses are less than the 0.5 quantile of uncertain responses. The top three turbulence parameters in sensitivity ranking are identical in various situations, namely the longitudinal turbulence intensity factor, longitudinal turbulence decay coefficient in the transverse direction, and longitudinal turbulence integral scale.

3. Surrogate-based rapid fragility assessment of super high-rise structures subjected to combined earthquake and wind hazards

This article presents a machine learning (ML)-based method for the rapid and accurate assessment of the vulnerability of super-high-rise structures (SHRSs) subjected to multiple disasters, including earthquakes and winds. Using a typical super-high-rise TV tower as a case study, numerous nonlinear finite element analysis (FEA) models were developed, incorporating both epistemic and aleatory uncertainties, to generate a dataset of maximum inter-storey drift ratios (MISDR) for the SHRSs. Based on this dataset, Extreme Gradient Boosting (XGBoost) was employed to build a model for predicting the structural MISDR under combined earthquake and wind load conditions. After parameter tuning**,** the XGBoost model demonstrated exceptional performance in predicting the structural MISDR values. Next, the Monte Carlo simulation (MCS) method was applied to joint earthquake-wind vulnerability analysis of the SHRSs, using the trained XGBoost metamodel. Additionally, the SHapley Additive exPlanations (SHAP) tool was employed to analyze the impact of various uncertainty parameters on the MISDR responses of the SHRSs. The results showed that combined loading scenarios produce the larger structural responses than the individual hazard scenarios; aleatory uncertainty parameters have a greater influence on the MISDR values than the epistemic uncertainty parameters; and seismic excitations influence the MISDR more significantly than the wind loads. Thus, the proposed XGBoost-based approach offers valuable support for quantifying uncertainties and efficiently assessing the

fragility of SHRSs under the multiple hazards. The main conclusions of this study are summarized as follows:

(1) The developed XGBoost demand metamodel performed well in rapidly predicting the MISDR responses across an ensemble of multi-hazards scenarios. This further facilitates fragility analysis associated with predefined damage states, achieving notably low prediction errors and computational costs. In addition, the structural and hazard load uncertainties can be considered using this surrogate model.

(2) The combination of earthquake and wind load scenarios resulted in a greater structural response than individual hazard scenarios. However, as the intensity of another hazard increases, the impact of the individual hazards diminishes. Furthermore, compared to wind loads, seismic excitations had a more significant impact on the MISDR of the SHRS.

(3) The coupled multi-hazards fragility estimates increase as the PGA and wind speed increase, and within the given multiple load intensity range, the seismic loads dominate the vulnerability of the SHRS. Moreover, the required PGA was inversely correlated with the wind speed for a given fragility probability.

(4) PGA, $\boldsymbol{\zeta}$, $\boldsymbol{f_c}$ and v_{10} are the four variables with the greatest impact among all the uncertainty parameters, which play a significant role in the MISDR values of the SHRS. Overall, the aleatory uncertainty parameters had a greater impact on the MISDR responses than the epistemic uncertainty parameters. For epistemic uncertainties, the ranking of the impact extent of parameter categories on MISDR is as follows: structural system parameters ($\boldsymbol{\zeta}$, $\boldsymbol{m_f}$), concrete material parameters ($\boldsymbol{f_c}$, $\boldsymbol{E_c}$), steel geometric parameters ($\boldsymbol{P_r}$, $\boldsymbol{P_t}$), steel material parameters ($\boldsymbol{f_y}$, $\boldsymbol{E_s}$), and concrete geometric parameter ($\boldsymbol{C_t}$). This highlights the critical need to account for stochastic variability in fragility assessments.

4. HybridAugment: a simple, effective and versatile automatic augmentation method for crack segmentation

Deep learning methods, such as the semantic segmentation, have shown excellent performance and good application prospects for detecting the cracks in infrastructure. However, the small sample size of published crack segmentation datasets, the high cost of labeled image acquisition and expansion have greatly limited the performance of the model. The data augmentation is an ideal method, however, in addition to the weak transferability of existing augmentation policies, the choice of augmentation policies often requires trade-off complexity, cost and performance. In this paper, an effective and versatile automatic augmentation method is presented for the crack segmentation, named HybridAugment (HA). The implementation of the HA needs to rely on the augmentation operation Mix-Crack and the augmentation selection method proposed here, but the entire process is parameter-free and cheap. To understand the crucial requirements for its performance, extensive ablation experiments are performed with different

operational designs, augmentation space sizes and samples. And then the HA compared with previous state-of-the-art methods in a variety of crack segmentation scenarios. The results have demonstrated that the HA outperformed previous augmentation policies, and achieved an excellent performance in terms of both in accuracy and stability.

Development of New Tools and Methodologies for Biomass Characterization

by Arthur Ragauskas, Member EUAS

Short Biography

Dr. Arthur Ragauskas held the first Fulbright Chair in Alternative Energy and is a Fellow of the 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 the 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 Energy and Environmental Sciences Directorate, Biosciences Division, at ORNL. His research program is directed at understanding and exploiting innovative sustainable bioresources for the circular economy. 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 are summarized in ***725 peer-reviewed*** *publications. His Fulbright-sponsored activities at the Chalmers University of Technology, Sweden were focused on 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 2014 ACS Affordable Green Chemistry Award, the 2017 AIChE Green Processing Award, the 2017 Academia Distinguished Service Award, 2019 AIChE Chase Award and 2022 RSC Environment, Sustainability, and Energy Division open award: Environment Prize. In addition, his students and postdocs have won several awards, including the ACS graduate research award, the ORNL UT-Battelle Award, and the ORNL Supplementary Performance Award.*

Dr. 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 the Journal of Chemical Technology and Biotechnology. Dr. Ragauskas has served on several advisory boards and review panels including the Austrian Science Fund, European Commission Research Directorate, National Science Academy, J. Paul Getty Trust, NSF, USDA, DOE, ARAPA-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.

Summary Statement: Ragauskas' Governor's Chair in Biorefining

Ragauskas heads a multifaceted program to understand and exploit the fundamental structure of municipal waste and bioresources to develop new and improved conversion pathways for sustainable fuels, power, materials, and chemicals within the circular economy while educating the next generation of leaders. The program leverages the unique research infrastructure and expertise located on the campuses of the Oak Ridge National Laboratory (ORNL), University of Tennessee, Knoxville (UTK), and the University of Tennessee Institute of Agriculture (UTIA). Ragauskas' research thrusts focus on four central overlapping focus areas:

- Fundamental investigation of the structure of lignocellulosics 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
- Upcycling of societal waste streams.

Ragauskas assumed the ORNL-UTK Governor's Chair in Biorefining in June 2014 and was renewed in October 2019. This UTK faculty position, jointly funded by UTK and ORNL, was envisaged to develop a fundamental research and academic program for sustainable biomass biorefining. His research-educational thrusts are pursued and developed within the boundaries of a circular economy.

Figure 1: Overview of Ragauskas' ORNL, UTK, and UTIA Governor Chair in Biorefining.

Historically, the bio-economy was frequently viewed from the "lens of biorefining bioresources from forest and agricultural resources" to serve society's needs, which by default are centered in major metropolitan centers. Over the last decade, this vision of producers and consumers has evolved, as captured by the circular economy (see **Fig. 1**), in which products are manufactured to be used, recycled, and reused. Thus, the bio-economy and Ragauskas' studies have been

broadened to utilize virgin biomass resources and waste streams from industry and the general population. The outcomes of Ragauskas studies over the past 4.5 years have been documented in +239 publications, three patent filings, +60 conference presentations, and the graduation of four UTK Ph.D. students. Reflective of these studies, Ragauskas has a Google H-Index of 128 and was the 2022 awardee of the *RSC Environment, Sustainability, and Energy Division open award: Environment Prize*.

Significant Research Contributions: To address evolving research and educational challenges in biorefining-circular economy, Dr. Ragauskas has developed a dynamic, internationally recognized ORNL-UTK-UTIA research team in the field of fundamental (i) biorefining of lignocellulosics, (ii) green chemistry/engineering, (iii) material science of bio-derived materials, and (iv) valorization of modern societal waste streams.

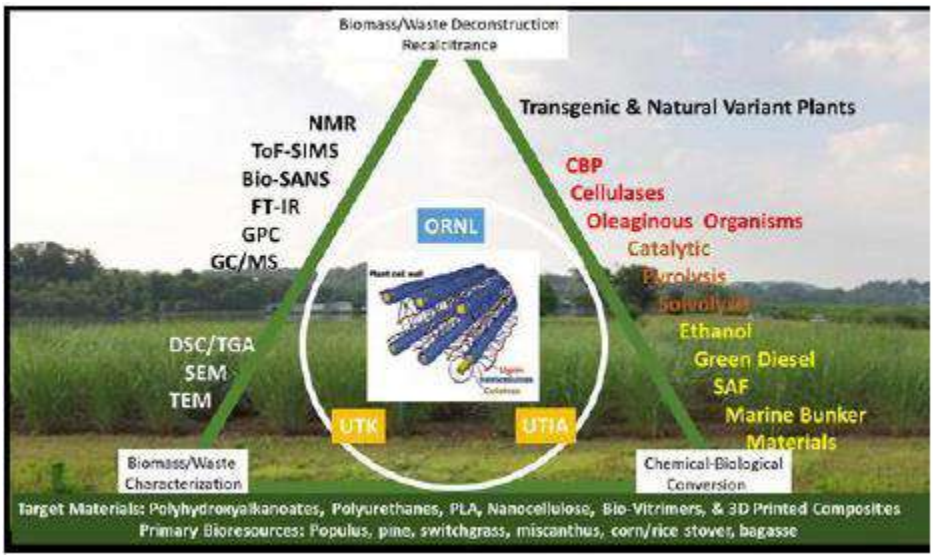

Figure 2: Ragauskas' biorefining studies.

Figure 2 demonstrates a strong emphasis on advanced analytics and biofuel research, which is consistent with Ragauskas' contributions to the Center of Bioenergy Innovation (CBI) and Science Focus Area (SFA, titled' Visualization of Solvent Disruption of Biomass and Biomembrane Structures in the Production of Advanced Biofuels and Bioproducts') DOE-funded programs centered at ORNL. As shown in **Figure 3**, our circular economy studies are primarily directed at upcycling waste streams for sustainable generation of chemicals, fuels, and materials. Both focus areas leverage ORNL, UTK, and UTIA research infrastructure and expertise. (NB: our coal material studies are directed at providing value-added alternatives to the combustion of coal)

Figure 3: Ragauskas' circular economy studies.

ORNL Focused Activities*:* Five selected publications representing Ragauskas' 2020-2024 Governor's Chair research efforts at ORNL are summarized below:

1. Economics and global warming potential of a *commercial*-scale delignifying biorefinery based on cosolvent-enhanced lignocellulosic fractionation to produce alcohols, sustainable aviation fuels, and biomass co-products. Klein, Bruno Colling; Scheidemantle, Brent; Hanes, Rebecca J.; Bartling, Andrew W.; Grundl, Nicholas J.; Clark, Robin J.; Biddy, Mary J.; Tao, Ling; Trinh, Cong T.; Guss, Adam M.; Wayman, Charles E.; Ragauskas, Arthur J.; Webb, Erin G.; Davison, Brian H.; Cai, Charles M., *Energy & Environmental Science* (2024), 17(3), 1202-1215.
2. Characterization and molecular simulation of lignin in cyrene pretreatment of switchgrass. Wang, Yun-Yan; Wang, Yunxuan; Liang, Luna; Smith, Micholas Dean; Meng, Xianzhi; Pu, Yunqiao; Mazarei, Mitra; Agarwal, Rupesh; Rukmani, Shalini J.; Davison, Brian H.; Ragauskas, Arthur J. *Green Chemistry* (2024), 26(6), 3170-3182
3. Novel candidate genes for lignin structure identified through genome-wide association study of naturally varying *Populus trichocarpa.* Bryant, Nathan; Zhang, Jin; Feng, Kai; Shu, Mengjun; Ployet, Raphael; Chen, Jin-Gui; Muchero, Wellington; Yoo, Chang Geun; Tschaplinski, Timothy J; Pu, Yunqiao; Ragauskas, Arthur J. *Frontiers in Plant Science* (2023), 14, 1153113.
4. Deconstruction of biomass enabled by local demixing of cosolvents at cellulose and lignin surfaces. Pingali, Sai Venkatesh; Smith, Micholas Dean; Liu, Shih-Hsien; Rawal, Takat B.; Pu, Yunqiao; Shah, Riddhi; Evans, Barbara R.; Urban, Volker S.; Davison, Brian H.; Cai, Charles M.; Ragauskas, Arthur J.; O'Neill, Hugh, M.; Smith, Jeremy; Petridis, Loukas. *Proceedings of the National Academy of Sciences of the United States of America* (2020), 117(29), 16776-16781.
5. Tensile properties of 3D-printed wood-filled PLA materials using poplar trees. Bhagia S; Lowden RR; Erdman D; Rodriguez M; Haga BA; Solano IRM; Gallego NC; Pu Y; Muchero W; Kunc, V; Ragauskas AJ. *Applied Materials Today* (2020) 21, 100832.

UTK/UTIA Focused Activities: In addition to these activities, Ragauskas has developed several UTK-UTIA research thrusts leveraging ORNL capabilities, as summarized in five representative publications presented below:

1. 3D printed lignin/polymer composite with enhanced mechanical and anti-thermal-aging performance. Zhang, Shuyang; Meng, Xianzhi; Bhagia, Samarthya; Ji, Anqi; Dean Smith, Micholas; Wang, Yun-yan; Liu, Bo; Yoo,

Chang Geun; Harper, David P.; Ragauskas, Arthur J. *Chemical Engineering Journal* (2024), 481, 148449.
2. Catalytic cascade upcycling single-use natural rubber glove wastes into fuels via a two-stage pressurized fixed-bed reactor. Wang, Jia; Jiang, Jianchun; Meng, Xianzhi; Lam, Su Shiung; Ragauskas, Arthur J.; Wang, Yanqin. *Fuel Processing Technology* (2022), 238, 107490.
3. Upcycling disposable face masks into fuel range iso-alkanes through hydropyrolysis coupled with vapor-phase hydrocracking. Wang, Jia; Jiang, Jianchun; Zhang, Yiyun; Meng, Xianzhi; Ragauskas, Arthur J. *Energy* (2023), 263(Part_B), 125843.
4. A facile strategy to fabricate a lignin-based thermoset alternative to formaldehyde-based wood adhesives. Shi, Xiaoyu; Gao, Shishuai; Jin, Can; Zhang, Daihui; Lai, Chenhuan; Wang, Chunpeng; Chu, Fuxiang; Ragauskas, Arthur J.; Li, Mi. *Green Chemistry* (2023), 25(15), 5907-5915.
5. Influence of plasticizers on thermal and mechanical properties of biocomposite filaments made from lignin and polylactic acid for 3D printing. Wasti, Sanjita; Triggs, Eldon; Farag, Ramsis; Auad, Maria; Adhikari, Sushil; Bajwa, Dilpreet; Li, Mi; Ragauskas, Arthur J. *Composites, Part B: Engineering* (2021), 205, 108483.

Research Projects and Five-Year Plan: Our research activities are forward-looking and directed at developing fundamental science and engineering to advance next-generation biorefining operations that address circular economy challenges. We have leveraged critical assets on the ORNL, UTK, and UTIA campuses to develop unique solutions and understanding of biomass and its conversion to biofuels, bio-based chemicals, and materials. These advances have come due to our partnerships with researchers from several departments, including:

- ORNL: Neutron Sciences, Chemical Sciences, BioSciences Division, Computational Systems Biology, and Manufacturing Demonstration Facility
- UTK: Chemical Biomolecular Engineering, Department of Plant Sciences
- UTIA: Center for Renewable Carbon

We remain one of the leading groups in biomass characterization and valorization of cellulose and lignin, both nationally and internationally. Based on our past accomplishments and ongoing research efforts, two Center proposals have been submitted to (1) NSF: Global Center for Sustainable Bioproducts and (2) DOE: Assessment of CORE-CM Resources in Eastern Coastal U.S. Waste Streams. We have been and will continue to strongly support ORNL's SFA and CBI's research mission, working with plant scientists and deconstruction teams to characterize and understand the key plant cell wall features that contribute to recalcitrance. In addition, as our nanocellulose/lignin and related material studies at UTK/UTIA mature, we anticipate leveraging ORNL's SNS, computational science, and plant science expertise in joint proposals. Indeed, recent and future RFPs/FOAS from DOE, USDA, and NSF are highly aligned with our current research programs.

Educational Mission

Although Ragauskas' current position does not require a teaching component, a core value of his academic mission 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 a cornerstone of his career objectives. These career objectives include the following.

- 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 the Center for Renewable Carbon.

- Recruit, educate, and develop the next generation of scientists who will be nationally and internationally recognized leaders in biorefining, green chemistry/engineering of biofuels, bio-derived materials, chemicals, and circular economy chemical processes.

Concluding Statement

In summary, since the beginning of Ragauskas' Governor's Chair position in the summer of 2014, his 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 (1) bio-renewables for Biorefining biomass to biofuels, bio-derived materials, chemicals, and (2) Circular Economy studies involving upcycling plastics, REE recovery, and utilization of coal as a material, at ORNL, UTK, and UTIA. His accomplishments to date attest to his success in accomplishing these goals.

Guided Wave-Based Defect Localization via Parameterized FRF-Based Reduced-Order Models

by Wieslaw Ostachowicz, Member EUAS

Short Biography

*Prof. Wiesław Ostachowicz (**ORCID**: 0000-0002-8061-8614) graduated from GUT, Gdańsk, Poland, with an MSc in Mechanical Engineering. He defended his PhD and DSc (in Mechanical Engineering). In 1989, he was nominated for the Professor position. He is a Member of the Polish Academy of Sciences (elected on December 1, 2016).*

Prof W. Ostachowicz has led dynamics research at the IMP PAN for over thirty-five years. He specialises in several important sub-disciplines, like structural health monitoring techniques, vibration control, structural dynamics, composite structures, multifunctional materials, smart materials and structures, and damage assessment of structures, working in these fields both theoretically and experimentally. His research focused on developing and using the Spectral Finite Element Method for damage assessment and smart materials applications. His research in guided wave propagation has aimed to develop numerous vibroacoustic–ultrasonic methods for damage detection using smart sensor technologies. Those methods have demonstrated effectiveness and sensitivity to small cracks in metallic and composite structures without restrictions on load, boundaries, temperature, or environmental conditions.

Presently, prof Ostachowicz is involved in work (as editor/associate editor) for the following journals: Mechanical Systems and Signal Processing (Elsevier), Structural Health Monitoring (SAGE Publications), Intelligent Material Systems and Structures (SAGE Publ.), Smart Materials and Structures (IOP Publ.), Editorial Board Member, Strain (Wiley), Jour. of Mechanical Engineering Science (SAGE Publications).

Prof. Ostachowicz supervised 16 PhD dissertations and reviewed several PhD theses and professorships in the United Kingdom, South Africa, the USA, Italy, France, Japan, Spain, Hong Kong, Singapore, Italy, Austria, Sweden, Australia, Lithuania and the Netherlands.

Prof. Ostachowicz has received several prestigious awards and distinctions, including the Medal of O.C. Zienkiewicz (2013), the Dragon–STAR Innovation Award (1st place), which confirmed cooperation between Poland (Polish Academy of Sciences) and China (Hohai University and The Hong Kong Polytechnic University) in 2015, the SHM Life Achievements Award (sponsored by Boeing Co.), Stanford University, USA (2019), and the Gold Medal "Sapientia et Veritas" (2023).

LIST OF PUBLICATIONS (2024)

1. Sieber, P, Agathos, K, Soman, R, Ostachowicz, W, Chatzi, E, *Guided Wave-Based Defect Localization via Parameterized FRF-Based Reduced-Order Models*, JOURNAL OF ENGINEERING MECHANICS, Vol.150, Issue 9, doi 10.1061/jenmdt.emeng-7766, Published, SEP **2024**.
2. Pau A., Ostachowicz W., Rizzo P., *Special issue on ultrasonic guided waves for structural health monitoring*, JOURNAL OF VIBRATION AND CONTROL, doi 10.1177/ 10775463241265659, JUL **2024**.

3. Ullah, S, Kudela, P, Ijjeh, AA, Chatzi, E, Ostachowicz, W, *Simulation of Full Wavefield Data with Deep Learning Approach for Delamination Identification*, APPLIED SCIENCES-BASEL, Vol. 14, Issue 13, doi 10.3390/app14135438, Published JUL **2024**.
4. Sha, GG, Xiao, W, Zuo, HF, Cao, MS, Radzieński, M, Ostachowicz, W., *Global-local damage localization and imaging in beam structures using laser-measured natural frequencies and guided wavefields*, MEASUREMENT, Vol., doi 10.1016/ j.measurement.2024.115061. Art. No. 115061, Published AUG **2024**.
5. Zhang Y., Radzieński M., Ostachowicz W., *Diagnostic-prognostic framework for assessing the health status of composite structures*, INTERNATIONAL JOURNAL OF MECHANICAL SCIENCES, Vol. 278, doi 10.1016/j.ijmecsci.2024.109461, Article No. 109461, Published OCT **2024**.
6. Xiao W., Sha G.G., Lu X.H., Zuo H.F.; Cao M.S., Soman R., Ostachowicz W., *Experimental and numerical studies on compressive failure behaviors of stepped-scarf repaired composite stiffened panels*, ENGINEERING FAILURE ANALYSIS, Vol. 163, Part A, doi 10.1016/ j.engfailanal2024.108458, Article No. 108458, Published SEP **2024**.
7. Xiao W., Sha G.G., Lu X.H., Zuo H.F., Cao M.S., Ostachowicz W., *Compressive failure analysis of composite honeycomb sandwich panels with impact damage and stepped-scarf repairs*, THIN-WALLED STRUCTURES, Vol. 201, Part B, doi 10.1016/j.tws.2024.112012, Article No. 112012, Published AUG **2024**.
8. Fiborek P., Soman R., Kudela P., Chatzi E., Ostachowicz W.M., *Wave propagation analysis in composite plate with clapping delamination based on spectral element method*, HEALTH MONITORING OF STRUCTURAL AND BIOLOGICAL SYSTEMS XVIII, Vol. 12951, doi 10.1117/12.3012456, Proceedings of SPIE, Article No., 129510 D, Published **2024**.
9. Patange A., Soman R., Pardeshi S., Kuntoglu M., Ostachowicz W., *Milling cutter fault diagnosis using unsupervised learning on small data: A robust and autonomous framework*, EKSPLOATACJA I NIEZAWODNOSC-MAINTENANCE AND RELIABILITY, Vol. 26, Issue1, doi 10.17531/ein/178274, Article No.178274, Published **2024**.
10. Sieber P., Agathos K., Soman R., Ostachowicz W., Chatzi E., *Towards an FRF-based parametric surrogate for guided wave-based evaluation in multiple defect scenarios*, HEALTH MONITORING OF STRUCTURAL AND BIOLOGICAL SYSTEMS XVIII, Vol. 12951, doi 10.1117/12.3009903, Proceedings of SPIE, Article No. 129510 C, Published **2024**.
11. Soman R., Peters K., Wandowski T., Ostachowicz W., *Improved Damage Mapping with Hyperbola Approach for Guided Waves Based Structural Health Monitoring Using Fiber Bragg Grating sensors*, 7th International Conference of Engineering Against Failure, Vol. 2692, doi 10.1088/1742-6596/2692/1/012022, Book Series, Journal of Physics Conference Series, Published **2024**.
12. Soman R., Yuan F.G., Ostachowicz W., *Damage detection in structures using SH waves sensed with FBG sensors*, Health Monitoring of Structural and Biological Systems XVIII Vol. 12951, doi 10.1117/12.3011183, Book Series, Proceedings of SPIE, Article No. 1295107, Published **2024**.
13. Xu W., Ji M.C., Cao M.S., Su Z.Q., Ostachowicz W., *Identification of local debonding in bolted panels using nonlinear pseudo-forces*, Health Monitoring of Structural and Biological Systems XVIII, Vol. 12951, doi 10.1117/12.3009653, Book Series, Proceedings of SPIE, Article No. 1295109, Published **2024**.
14. Zhang Y., Radzieński M., Ostachowicz W., *Effect of bending modes on failure analysis of adhesively bonded composite structures*, Health Monitoring of Structural and Biological Systems XVIII, Vol. 12951, doi 10.1117/12.3009665, Book Series, Proceedings of SPIE, Article No. 1295104, Published **2024**.
15. Zhang Y., Radzieński M., Xue S., Wang Z., Ostachowicz W., *A method for detecting cracks on the trailing edge of wind turbine blades based on aero acoustic noise analysis*, Structural Health Monitoring-an International Journal, doi: 10.1177/14759217241303452, DEC **2024**.
16. Sikdar S., Ostachowicz W., *Bonded repairs: enhancing structural integrity and sustainability of composite materials*, Proc. of the ASME 2024, 51st Annual Review of Progress in Quantitative Nondestructive Evaluation QNDE 2024, Denver, Colorado, July 22-24, **2024**.
17. Zhang Y., Radzieński, Wiesław Ostachowicz, *Methods for remaining useful life prognosis of adhesively bonded composite structures*, Proc. of the ASME 2024, 51st Annual Review of Progress in Quantitative Nondestructive Evaluation QNDE 2024, Denver, Colorado, July 22-24, **2024**.

18. Kudela P., Fiborek P., Ostachowicz W., *Wave propagation for structural health monitoring (WaveProSHM): open software with GUI*, 11th European Workshop on Structural Health Monitoring (EWSHM 2024), Potsdam, Germany, June 10-13, **2024**.

A method for detecting cracks on the trailing edge of wind turbine blades based on aeroacoustic noise analysis

Abstract: This study uses aero acoustic noise to identify cracking and debonding faults on the trailing edge (TE) of wind turbine blades, which is very meaningful because it can monitor early faults without affecting the normal operation of the wind turbine, thereby improving the safety and reliability of the wind turbines and extending the service life of the blades. First, the semi-empirical model, NAFNOISE, is used to analyse the factors that influence the noise from the TE, such as chord length, angle of attack, and TE thickness. Computational aeroacoustics (CAA) as a more precise finite element method is further employed to calculate the areo acoustics noise (AAN) of the blade with TE cracking. Based on the vortex shedding diagram of the calculation results, a preliminary explanation is provided for the main reason high-frequency energy appears in the sound power spectrum when the blades have a TE cracking failure. Next, the semi-empirical model is compared with the noise waveforms obtained by CAA, the differences between different models in identifying TE cracking are analysed, and the theoretical acoustic characteristics of AAN changes when blades fail are drawn. Finally, a noise detection experiment and corresponding signal processing technology are discussed. The results demonstrate that the method proposed in this article is capable of detecting debonding and cracking faults at the TE and improves the theoretical research on active and noncontact damage monitoring of the blades.

Simulation of Full Wavefield Data with Deep Learning Approach for Delamination Identification

Abstract: In this work, a novel approach of guided wave-based damage identification in composite laminates is proposed. The novelty of this research lies in the implementation of ConvLSTM-based autoencoders for the generation of full wavefield data of propagating guided waves in composite structures. The developed surrogate deep learning model takes as input full wavefield frames of propagating waves in a healthy plate, along with a binary image representing delamination, and predicts the frames of propagating waves in a plate, which contains single delamination. The evaluation of the surrogate model is ultrafast (less than 1 s). Therefore, unlike traditional forward solvers, the surrogate model can be employed efficiently in the inverse framework of damage identification. In this work, particle swarm optimisation is applied as a suitable tool. The proposed method was tested on a synthetic dataset, thus showing that it can estimate the delamination location

and size with reasonable accuracy. The test involved complete wavefield data in the objective function of the inverse method, but it should also be underlined that partial data with measurements can be implemented. This is extremely important for practical applications in structural health monitoring, where only signals at a finite number of locations are available.

Compressive failure analysis of composite honeycomb sandwich panels with impact damage and stepped-scarf repairs

Abstract: Composite honeycomb sandwich panels (CHSPs) have been widely used in the aerospace industry owing to their lightweight and superior mechanical properties. However, these CHSPs are susceptible to impact damage, significantly reducing compressive strength and potentially jeopardising aircraft safety. It is crucial to investigate repair methods for CHSPs with impact damage. This paper aims to evaluate the repair performance of CHSPs with impact damage by analysing their compressive failure behaviours. To accomplish this, both experimental tests and advanced numerical models are employed. The numerical models for the intact, damaged and stepped scarf-repaired CHSPs are established using the progressive failure analysis model, cohesive zone model and sandwich plate theory. A good agreement is observed between the experimental results and numerical predictions of compressive failure behaviours. Moreover, the validated numerical models are successfully utilised to determine optimum repair parameters by parametric analysis of the repaired CHSPs. Establishing these numerical models offers an accurate and cost-effective evaluation of repair performance for CHSPs with impact damage, highlighting the novelty and main contribution of this paper.

Identification of local debonding in bolted panels using nonlinear pseudo-forces

Abstract: Bolt looseness can occur and is subject to long-term structural service. With this concern of structural integrity and safety, there is a considerable demand to identify bolt-looseness-caused local debonding in connected structural components such as bolted panels. With non-contact laser scanning, transverse Operating Deflection Shapes (ODSs) of a bolted panel can be measured with high spatial resolutions. Perturbation to the linear transverse dynamic equilibrium of the panel can be regarded as the Linear Pseudo-Force (LPF), which is applied to the debonding region only and vanishes at undamaged locations. However, nonlinearities caused by contact of debonding interfaces during vibrations are not considered in the LPF model. Therefore, only linear damage features can be

contained in the LPFs established on linear ODSs, leading to incompleteness of damage features. Addressing this problem, this study demonstrates a Nonlinear Pseudo-Force (NPF) model from the nonlinear transverse motion equation of a beam-type bi-layer panel model with local debonding. Superior to LPFs, NPFs can extract linear and nonlinear damage features from linear and nonlinear ODSs, respectively. Like LPFs, NPFs concentrate in the debonding regions to form local peaks. Therefore, the NPF can be an ideal nonlinear indicator for identifying local debonding in bolted panels. The applicability of the NPF is experimentally validated by identifying width-through debonding in a steel panel connected by bolts, whose ODSs at linear and nonlinear (higher) harmonics are acquired through non-contact laser scanning measurement. Experimental results reveal that the NPF can extract complete linear and nonlinear damage features and hence has a higher-dimensional capacity for identifying local debonding in connected structural components, such as bolted panels, whose occurrence, location, and size can be graphically characterised.

Damage detection in structures using SH waves sensed with FBG sensors

Abstract: To perform active structural health monitoring (SHM), Guided waves (GW) have received significant interest as they can inspect large areas with a few sensors and are sensitive to barely visible structural damages. Fiber Bragg grating (FBG) sensors offer several advantages, but their use has been limited for GW sensing due to their limited sensitivity. FBG sensors in the edge-filtering configuration have overcome this issue with sensitivity, and there is a renewed interest in their use. In addition, the FBG sensors can sense the shear horizontal (SH wave) when deployed perpendicular to the propagating wave. The SH_0 wave is non-dispersive and hence simplifies the signal processing. As a result, the SH_0 wave may improve the quality of damage detection and localisation. Thus, this paper investigates the use of SH_0 waves sensed using FBG sensors in an edge-filtering configuration. The SH wave is generated using d36-based piezo actuators and sensed using FBG sensors. The method is developed for a simple aluminium plate with simulated damage scenarios. The process shows promising results and can potentially be used for reference-free damage detection.

Activities in Materials Science and Engineering

by Derek O. Northwood, Member EUAS

Short Biography

Professor Derek O. Northwood is a Distinguished University Professor Emeritus 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 715 papers in refereed international journals and conference proceedings, 9 chapters in books and has edited 10 books, on a wide range of topics including materials and their applications, and engineering and technology education. He has been elected Fellow of six 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); and Fellow of Alpha Sigma Mu (FAΣM), The International Professional Honor Society for Materials Science and Engineering. In 2024, Professor Northwood was recognized again as being among the world's top 100,000 - or top 2% of scientists - according to the database published by Stanford University. Professor Northwood continued in his role as Associate Editor of both the Global Journal of Engineering Education and World Transactions on Engineering and Technology Education, and Editorial Board Member (Hydrogen and Fuel Cells) for Renewable Energy.

RESEARCH ACTIVITIES AND PUBLICATIONS 2024

As in 2023, my principal research activities have been conducted in cooperation with Professor Cheng Liu at Yangzhou University, China and Dr. Hao Ma, and associated researchers, at BGRIMM Technology Group, Beijing, China.

The cooperative work with Professor Cheng Liu at Yangzhou resulted in one publication in 2024, on sequential solution annealing of a CrMnCN austenitic stainless steel. A sequential solution annealing treatment was designed to dissolve carbide and nitride precipitates and thereby produce a steel with a higher impact energy.

Liu, W., Northwood, D.O., Ding, G., Liu, C.

Sequential solution annealing of a CrMnCN austenitic stainless steel (2024) *Journal of Materials Research and Technology* , 31, pp. 1871-1884

The influence of various solution annealing treatments on the microstructure and mechanical properties of a new Cr–Mn austenitic stainless steel with 1.15 wt% (C + N) and 0.51 C/N ratio has been investigated. A sequential solution annealing (SSA) treatment is designed to sufficiently dissolve and lower numerous precipitates including carbides and nitrides in the austenite matrix. In this process, the hot-forged steel is firstly solution heat treated at 1120 °C for 2 h, then continuously heated to 1180 °C for 0.5 h, and further heated to 1200 °C for 0.5 h, followed by water quenching. The experimental results show that the austenite grain size increases, and number of precipitates decreases, with increasing temperature and time of solution annealing treatments. The highest impact energy is obtained after this SSA treatment due to a more homogeneous grain distribution, a smaller amount of carbides remaining on the grain boundary, and solid solution strengthening of interstitial (C + N) atoms.

The research collaboration with Dr. Hao Ma on the recovery of valuable metals from ores and refractory concentrates has continued, and new work has been initiated on surface modification of calcined kaolinite particles and their incorporation into a polymer-polymer composite. There have been a total of 6 publications in 2024.

Yuan, Y., Tang, X., Shi, J., Zhou, C., Li, L., Sun, H., Northwood, D.O., Waters, K.E., Ma, H.

Controlling and Tuning the Dispersion Properties of Calcined Kaolinite Particles in Various Organic Solvents via the Modification Method Using Triethoxyvinylsilane and 3-Mercaptopropionic Acid
(2024) *Molecules*, 29(17), 4129

The surface of calcined kaolinite particles underwent chemical modification using Vinyltriethoxysilane (VTMS) and 3-mercaptopropionic acid (3-MPA). The grafting ratio of VTMS on the calcined kaolinite surface was adjusted by varying its quantity. FT-IR analysis revealed the initial grafting of VTMS onto the kaolinite

surface, resulting in the formation of a C=C reactive site on the surface. Subsequently, an olefin click reaction with 3-MPA occurred, leading to the effective grafting of 3-MPA onto the kaolinite surface and the formation of an efficient coating. Thermal analysis indicated that the optimal grafting level was kaolinite surface was approximately 40% when V:K was 0.5. Water contact angle and dispersion experiments demonstrated that the surface properties of kaolinite were effectively controlled by this modification approach. At V:K = 0.3, the modified kaolinite particles exhibited good dispersion in both polar and non-polar solvents. In polar solvents, the average particle size of modified kaolinite was below 1100 nm, while in non-polar solvents, it did not exceed 5000 nm. Considering all aspects, a V:K ratio of 0.3 is recommended. Further investigation into the impact of adding 3-MPA on the surface properties of modified kaolinite particles based on V:K = 0.3 revealed that the hydrophilicity of the modified particles could be enhanced. However, it is advised to keep the maximum M:V ratio (3-MPA to kaolinite) at 1.0.

Yuan,Y., Tang,X., Sun, H., Shi, J. Zhou,C., Northwood, D.O.., Waters, K.E., Ma, H.

Surface Modification of Calcined Kaolinite for Enhanced Solvent Dispersion and Mechanical Properties in Polybutylene Adipate/ Terephthalate Composites
(2024) *Molecules*,11, 29(16), 3897

In order to regulate the surface properties of calcined kaolinite for the purpose of achieving uniform distribution within various polar dispersion media, 3-aminopropyltriethoxysilane and phenyl glycidyl ether were employed to chemically modify calcined kaolinite. The grafting rate, surface properties, and dispersion properties of calcined kaolinite particles in different polar organic media were changed by varying the dosage of the modifiers. FT-IR analysis confirmed successful surface modification, while thermogravimetric analysis indicated a maximum graft coverage of 18.44 μmol/m2 for the modified particles. Contact angle measurements and particle size distribution analyses demonstrated the effective adjustment of surface characteristics by the modifiers. Specifically, at a mass ratio of 1.0 of modifier to kaolinite particles, the modified particles exhibited a contact angle of around 125°, achieving uniform dispersion in different polarity media. Particle size distribution ranged from 1600 nm to 2100 nm in cyclohexane and petroleum ether, and from 900 nm to 1200 nm in dioxane, ethyl acetate, and DMF, showcasing a significant improvement in dispersion performance compared to unmodified particles. Concurrently, to improve the mechanical properties of

PBAT, modified particles were incorporated into the PBAT matrix, and the effect of modified particle addition on the tensile strength and fracture tensile rate of the composites was investigated. The optimal amount of modified particles is 6 wt.%~8 wt.%. This article aims at synthesizing modifier molecules containing different hydrophilic and hydrophobic groups to chemically graft onto the surface of calcined kaolinite. The hydrophilic and hydrophobic groups on the modified particles can adapt to dispersed systems of different polarities and achieve good distribution within them. The modified particles are added to PBAT to achieve good compatibility and enhance the mechanical properties of the composite material.

Qin, S., Yang, B., Northwood, D.O.., Waters, K.E., Ma, H.

The Deep Removal of Mercury in Contaminated Acid by Colloidal Agglomeration Materials M201
(2024) *Minerals*,14(8), 782

The high-temperature roasting/smelting process of copper and zinc concentrates will cause the mercury in the concentrate to evaporate into the flue gas, and most of the mercury in the flue gas will eventually enter the waste acid in its ionic form. A highly efficient mercury removal agent M201 with long carbon chains and loaded active functional groups can adsorb and disperse fine particles for mercury removal in the system. Through bridging, the linear structure is woven into a network to achieve large-scale capture and dispersion of fine particles and colloidal substances. The recommended operating conditions for developing mercury deep purification technology are as follows: M201 reagent concentration of 50 g/L, 6 mL/L added acid solution, room temperature, mixing time of 5 min, air flotation time of 10 min, ventilation rate of 0.1 L/min, H2SO4 concentration of 33.67 g/L, and the residual mercury content of 2 mg/L (the mercury content reaches 0.01 mg/L after two-stage mercury removal treatment). Meanwhile, the residual arsenic content is 21.9 mg/L. This study shows a better separation of arsenic and mercury and achieves one-step mercury removal.

Xu, J., Qin, S., Zheng, C., Sun, H., Yang, B., Liu, S. Qiu, G., Northwood, D.O.., Waters, K.E., Ma, H.

Study on Column Leaching Behavior of Low-Grade High Calcium and Magnesium Copper Ore
(2024) *Minerals*, 14(8), 822

This paper studies the process mineralogy, mechanism, and kinetics of column leaching behavior of low-grade high-calcium–magnesium copper ore. The effect of sulfuric acid concentration, leach solution spraying intensity, and material particle size on column leaching kinetics is discussed. The kinetic analysis of column leaching of copper indicates that sulfuric acid concentration has a significant impact. As sulfuric acid concentration increases, the limiting step of reaction shifts from chemical reaction control to a combination of chemical reaction and diffusion mixing control. Spraying intensity also affects copper column leaching; increasing intensity shifts the limiting step from diffusion control to mixing control, thereby mitigating the effects of diffusion control. Regarding other elements, it is found that iron leaching is primarily controlled by chemical reaction, while calcium leaching is mainly controlled by chemical reaction. As sulfuric acid concentration increases from 10 g/L to 20 g/L, the limiting step for calcium leaching shifts from chemical reaction control to chemical reaction and diffusion-mixing control.

Yang, B., Song, B., Chen, L., Sun, H., Northwood, D.O.., Waters, K.E., Ma, H.

Influence of Top Slag containing TiO2 and VOx on Hot Metal pre-Desulfurization
(2024) *Metals*, 14(8), 910

Abs The desulfurization capacity of top slag in the process of pre-desulfurization of hot metal containing vanadium and titanium was researched. The top slag system of CaO-SiO2-MgO-Al2O3-TiO2-VOx that was formed by blast furnace slag and a CaO desulfurization agent reduced the sulfur in hot metal from 0.08 wt.% to 0.02 wt.%. It was found that the resulfurization of the slag happened in the later periods of the desulfurization process. The vanadium–titanium oxides were both acidic in the desulfurization slag. TiO2 and VOx reacted with the basic oxides to form CaTiO3 and MgV2O4 at 1623 K, which reduced free CaO and was not conducive to top slag desulfurization. The results of calculation showed that the top slag desulfurization accounted for 15% of the total desulfurization. Using the ionic and molecule coexistence theory of slag structure, it is shown that the desulfurization efficiency could be enhanced by adjusting both the amount of desulfurization agent and the composition of the blast furnace slag before pre-desulfurization.

Sun, K., Jie, X., Zhang, Y., Gao, W., Northwood, D.O., Waters, K.E., Ma, H.

Analysis of the Feeding Behavior in a Bottom-Blown Lead-Smelting Furnace
(2024) *Metals*, 14(8), 906

Computational fluid dynamics (CFD) software was used to simulate the feeding behavior in a bottom-blown lead-smelting furnace. The results show that when the particle size is less than 30 μm, 20% of the particles are suspended in the gas phase and do not enter the melt pool for smelting, thus resulting in material loss. When the particle size exceeds 75 μm, the particles settle in the metal layer. When the particle size is 40–60 μm, the particles are distributed in the slag and metal phases, and the material is uniformly distributed in the molten pool; additionally, the average velocity of the particles exceeds 1.4 m/s, the average temperature exceeds 960 K, and the particles exhibit better behavior within this range, thus rendering it the optimal range of particle sizes for feeding.

Stochastic Finite Element Method & Numerical Modeling of Random Composites

by Marcin Kamiński, Member EUAS

Short Biography

Prof. Marcin Kamiński has been a full professor in the Department of Structural Mechanics, Łódź University of Technology since 2015 and now He is the Head of the Discipline Civil Engineering, Geodesy & Transportation in the Faculty of Civil Engineering, Architecture & Environmental Engineering since 2019. He worked before in Division of Mechanics of Materials (1994-2009), was the Head of Department of Steel Structures (2010-2013); then He joined Department of Structural Mechanics as the Head of Division of Structural Reliability.

His main research includes the Stochastic Finite Element Method (and some other discrete stochastic numerical methods), numerical modeling of random composites including homogenization theory, reliability assessment and optimization of civil engineering structures, stochastic ageing processes, and also recently - an application of probabilistic entropy in engineering computations (in the framework of the research grant OPUS no. 2021/41/B/ST8/02432 sponsored by the National Science Center in Cracow, Poland).

He spent a postdoctoral study at Rice University in Houston, TX, USA, was a visiting professor at Leibniz-Institute of Polymer Research in Dresden, Germany, and also at Politecnico di Milano, Italy. He authored more than 200 research papers in various journals including International Journal for Numerical Methods in Engineering, Composite Structures, International Journal of Solids & Structures, and also Computers & Structures. He published two monographs: "Computational Mechanics of Composite Materials", Springer, 2005, and also "The Stochastic Perturbation Method for Computational Mechanics", Wiley, 2013. He serves as the associate editor in Mechanics Research Communications (by Elsevier, since 2013) and the member of editorial board in International Journal for Numerical Methods in Engineering (Wiley), Acta Mechanica (Springer), Computers & Structures (Elsevier), Journals of Composites Science, and also SCI (MDPI).

He was the recipient of the fellowships from Foundation for Polish Science (1996 & 1999), J. Argyris Award from ECCOMAS and Elsevier (2001), J.T. Oden Scholarship at The University of Texas (Austin, TX, USA, 2004), and also some Polish national or academic awards including Bronze Cross of Merit (1998), Silver Cross for the Longstanding Service (2017), Medal of Commission of Education (2022), and also very recently The Research Prize of Ministry of Education & Science in 2023. He has been recognized recently (since 2021) as the World's Top 2% Scientists by Stanford University, CA, USA.

Prof. M. Kamiński teaches mainly the courses relevant to Structural Reliability, Optimization & Parametric Design and Finite Element Method, but also various courses related to Steel Structures, Strength of Materials and Theoretical Mechanics. He coauthored (with prof. B. Rogowski) the academic textbook "Technical Mechanics" having two editions – in 2009 & 2013. He taught in His career many academic courses for Civil Engineering, Environmental Engineering, Architecture & Architecture Engineering. He served as the promoter for 8 Ph.D. theses as well as for more than 40 M.Sc. and B.Sc. students.

Mechanics Research Communications paper (2025):

This study is devoted to the development of effective mechanical properties for some specific cellular materials with hexagonal structures exhibiting uncertain imperfections in their internal geometry. Analytical formulas for the first four probabilistic moments and relative entropies are developed for the effective Young modulus and yield strength. A numerical simulation is presented to show a comparison of these formulas with the results obtained via the Monte-Carlo simulation and the generalized stochastic perturbation technique. Three different entropy measures proposed by Bhattacharyya, Kullback-Leibler, and Hellinger are used to quantify probability distributions of these two characteristics for the cellular material skeleton and the corresponding effective parameters of the entire structure. This methodology can be applied to a wide range of cellular materials, in which analytical formulas can be developed, and for case studies where the Finite Element Method (FEM) is used to determine the effective characteristics of such materials.

Computers & Structures (2024):

The main research problem studied in this work is an uncertain response and reliability assessment of the spatial cable structures due to the environmental stochasticity as well as material and geometrical imperfections. Some popular cable structures are analyzed for this purpose using the Stochastic Finite Element Method (SFEM) implemented with the use of three different techniques, namely the iterative generalized perturbation method, semi-analytical approach as well as the Monte-Carlo simulation. Uncertainty quantification delivered in this study is based on the series of FEM analyses of both static and dynamic structural problems. They enable the Least Squares Method determination of the structural polynomial responses linking extreme stresses and deformations with several uncorrelated uncertainty sources. Reliability assessment, fundamental in durability and Structural Health Monitoring, is completed using a comparison of the First Order Reliability Method (FORM) with probabilistic distance formulated by Bhattacharyya. Input uncertainties are assumed to be Gaussian according to the Maximum Entropy Principle. They have specific expected values following engineering design demands or the provisions of designing codes, whereas their standard deviations do not exceed the 10% level. The methods presented and the results obtained in this study may serve for further reliability analyses of large-scale civil engineering structures completed with both steel cables and also reinforced concrete plates like suspended bridges, for instance.

Computer Methods in Applied Mechanics and Engineering (2024):

The main idea of this work is to investigate the uncertainty propagation while homogenizing the periodic fiber-reinforced composites with some structural interface imperfections, and specifically their thermal and mechanical properties in linear elastic regimes. The effective modules method is implemented here with the use of two alternative Finite Element Method (FEM) programs based on its displacement (temperature) formulation. Probabilistic (Shannon) entropy and probabilistic distance are engaged here to quantify uncertainty propagation of effective characteristics as well as their probabilistic distance to the original composite's characteristics. Probabilistic entropies fluctuations are contrasted with the traditional moments-based approach while increasing the input statistical scattering of material characteristics. According to the Maximum Entropy Principle Gaussian input parameters are tested as inducing the largest deviations in

effective characteristics, but they are compared against some other symmetric distributions. The entire methodology is based upon the response random polynomials relating homogenized characteristics with material and geometrical parameters of the original composites subjected to randomization. Some series of the FEM experiments serve as the basis for the artificial neural network identification and optimization of these polynomials, whose application in conjunction with the Monte-Carlo simulation enables Shannon entropy determination. Relative entropy as well as the referential probabilistic moments are computed using the iterative generalized stochastic perturbation technique as well as the semi-analytical probabilistic method.

International Journal for Numerical Methods in Engineering (2024):

The generalized iterative stochastic perturbation approach to the stress-based Finite Element Method has been proposed in this work. This approach is completed using the complementary energy principle, Taylor expansion of the general order applicable to all random functions and parameters as well as nodal polynomial response bases determined with the use of the Least Squares Method. The main aim of this elaboration is the usage of such a probabilistic approach to determine Bhattacharyya relative entropy for some nonlinear engineering stress analysis with uncertainty. Mathematical apparatus with its numerical implementation has been used to study elastoplastic torsion of some prismatic bar with Gaussian material uncertainty and the corresponding reliability measures. This problem has been solved using the Constant Stress Triangular (CST) plane finite elements, the modified Newton–Raphson algorithm, whereas the first four probabilistic characteristics resulting from the iterative generalized stochastic perturbation method have been contrasted with these obtained with the crude Monte-Carlo sampling and the semi-analytical probabilistic approach.

Probabilistic Engineering Mechanics (2023)

The main objective of this work is to investigate natural vibrations of the thin (Kirchhoff-Love) plate resting on time-fractional viscoelastic supports using the Stochastic Finite Element Method (SFEM). The mechanical behavior of the supports is deterministic and is described by the fractional order derivatives of the Riemann-Liouville type. A subspace iteration method in conjunction with the continuation method is the basis of the numerical solution carried out using the displacement formulation of the Finite Element Method. The probabilistic analysis includes independent Monte-Carlo simulation, the semi-analytical approach, and the iterative generalized stochastic perturbation method of the first two probabilistic moments. Moreover, a corresponding relative entropy and the entropy-based reliability index are contrasted with the First Order Reliability Method (FORM). It has been found that the relative entropy for analyzed eigen-vibrations is some interesting alternative to the FORM methodology in reliability assessment.

Computer Methods in Applied Mechanics and Engineering (2023):

The main aim of this work is to present a numerical analysis of convergence and accuracy of the selected generalized perturbation-based schemes in linear and nonlinear problems of solid mechanics. An algorithm for determining the basic probabilistic characteristics has been developed using the iterative generalized stochastic higher-order perturbation method adjacent to symmetrically truncated Gaussian random variables. It has been confirmed that

usage of a sufficiently high order of the Truncated Iterative Stochastic Perturbation Technique (TISPT) allows for achieving any desired accuracy in determining up to the fourth-order probabilistic characteristics of static structural response. The semi-analytical probabilistic approach is the reference solution in this study, which is based upon the same composite response functions determined with the use of the Least Squares Method created using specific series of FEM experiments. The entire methodology has been provided for the given extreme value of the coefficient of variation α_{max} of the input uncertainty source. On the other hand, a selection procedure of the stochastic perturbation method order to achieve 1% numerical accuracy in all up to the fourth-order probabilistic moments has been proposed. Computational experiments include simply supported elastic Euler–Bernoulli beam, a set of steel diagrid structures, nonlinear tension of steel round bar as well as homogenization procedure of some particulate composite.

Engineering Analysis with Boundary Elements (2022):

The main objective in this work is to study an application of the Stochastic Boundary Element Methods implemented due to three different probabilistic approaches to analyze stability of the rectangular thin elastic and isotropic plates. This is completed with the use of polynomial approximations applied for the Least Squares Method recovery of critical forces resulting from some material and geometrical random imperfections in the plate, e.g. Young's modulus, Poisson's ratio, thickness. A deterministic core for solving the plate stability problem is the Boundary Element Method in direct approach and modified formulation of the boundary and domain integral equations. Probabilistic approaches employed here include traditional Monte-Carlo simulation, the semi-analytical approach as well as the iterative generalized stochastic perturbation method. Stochastic response in the form of up to the fourth order characteristics are studied numerically in addition to the input uncertainty level.

International Journal for Numerical Methods in Engineering (2021):

This paper considers the problem of determining probabilistic entropy fluctuations, which are important for understanding uncertainty propagation in mechanical systems in the elasto-plastic regime. Probabilistic entropy is conceptualized based on an initial definition by Shannon, which demands discrete representation of the uncertainty source. Numerical analysis is performed using the Response Function Method with polynomial bases. Coefficients are found and order optimization is completed using polynomial interpolations or the Least Squares Method. Approximations are based on the Finite Element Method. Local polynomial bases enable nonlinear increment analysis, and allow for a given degree of freedom in the FEM model to be described as a function of a random input parameter. Academic FEM software and the ABAQUS system were used for numerical experiments. Polynomial approximations, probabilistic moment computations, and statistical entropy estimations were programmed in the symbolic algebra package MAPLE. Transformation of the input probability density into the output function was performed using the Monte-Carlo simulation algorithm for statistically optimized polynomial bases of extreme displacement functions. Two computational examples are given to demonstrate probabilistic entropy fluctuations for a small statically indeterminate aluminum truss structure and also for practical engineering case study of the steel round bar under uniform tensile stress. In these examples, some material and geometrical uncertainties distributed

according to Gaussian, triangular, uniform as well as lognormal distributions were analyzed. The presented approach could be used for constitutive models of solids, computational fluid dynamics, and in other discrete numerical methods.

Journal of Constructional Steel Research (2018):

The main aim of this paper is to present a reliability estimation procedure for steel lattice telecommunication towers based on tensioned joint reliability. The experiment, which involved doing a full-scale pushover test of a 40 m high lattice tower, constituted the starting point for further analyses. Experimental data served as bases for finite element model calibration and assignment of steel mechanical properties based on tensile tests. A computational investigation was performed for random wind loads. Numerical considerations included a detailed dynamic analysis with respect to the specific wind velocity–time function, modeling of two particular tower joints by shell finite elements, and elastic-plastic range determination of joint reliability using the first-order and second-order reliability methods.

Acta Mechanica (2018):

The main objective is to investigate an effect of anisotropic distribution of the reinforcing particles in a cubic representative volume element (RVE) of the carbon–polymer composite including stochastic interphases on its homogenized elastic characteristics. This is done using a probabilistic homogenization technique implemented using a triple approach based on the stochastic perturbation method, Monte Carlo simulation as well as on the semi-analytical approach. On the other hand, the finite element method solution to the uniform deformations of this RVE is carried out in the system ABAQUS. This composite model consists of two neighboring scales–the micro-contact scale relevant to the imperfect interface and the micro-scale—having 27 particles inside a cubic volume of the polymeric matrix. Stochastic interface defects in the form of semi-spheres with Gaussian radius are replaced with the interphase having probabilistically averaged elastic properties, and then such a three-component composite is subjected to computational homogenization on the microscale. The computational experiments described here include FEM error analysis, sensitivity assessment, deterministic results as well as the basic probabilistic moments and coefficients (expectations, deviations, skewness and kurtosis) of all the components of the effective elasticity tensor. They also include quantification of anisotropy of this stiffness tensor using the Zener, Chung–Buessem and the universal anisotropy indexes. A new tensor anisotropy index is proposed that quantifies anisotropy on the basis of all not null tensor coefficients and remains effective also for tensors other than cubic (orthotropic, triclinic and also monoclinic). Some comparison with previous analyses concerning the isotropic case is also included to demonstrate the anisotropy effect as well as the numerical effort to study randomness in composites with anisotropic distribution of reinforcements and inclusions.

New Paradigm for Tracking Emotions

by Fuji Ren, Member EUAS

Short Biography

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.

1. INTRODUCTION

Emotion profoundly influences human communication and decision-making. In recent years, artificial intelligence systems that detect and respond to emotions have advanced significantly, enabling intelligent tutoring platforms, affective computing in games, and social robotics [1]–[3]. Although current methods achieve high accuracy for static classification of emotion from facial expressions, prosody, or text sentiment [4], they often overlook how affect evolves over time [5].

We observe that most pattern-recognition models effectively capture what can be called *external emotional energy* (EEE): the short-term, observable cues in speech or facial

gestures. However, such external signals do not necessarily reflect the actual underlying emotion [6], which involves deeper mental processes. Consequently, equating observable cues with genuine affective states can hinder performance in multi-label or time-extended contexts [7], [8].

To address this limitation, we propose the **Evolutionary Mental State Transition Model** (EMSTM). As shown in Figure 1, EMSTM operates in two major steps:

1) **Multi-modal EEE Extraction**: We fuse features from text, vision, and acoustics using cross-attention blocks, transforming them into an n-dimensional vector E_t representing external emotional signals.

2) **Mental state transition network (MSTN)**: We define a hidden emotional state $e_t \in \mathrm{R}^n$ that genuinely cor- responds to a user's internal affect. MSTN updates e_t from e_{t-1} under the influence of E_t, thereby modeling the time-varying nature of emotion.

We apply EMSTM to two multi-label benchmarks: CMU- MOSEI [9], a multi-modal dataset, and Ren-CECps [10], a large Chinese text dataset. Comparative experiments demonstrate that MSTN-based transitions outstrip purely static classification approaches, especially for majority emotion categories. The model remains computationally efficient, as transitions operate on a modest n-dimensional latent state rather than large recurrent or transformer stacks. This framework is grounded in the notion that observable outward signals (EEE) do not equate to the full emotional reality, aligning with dynamic psychological perspectives [6].

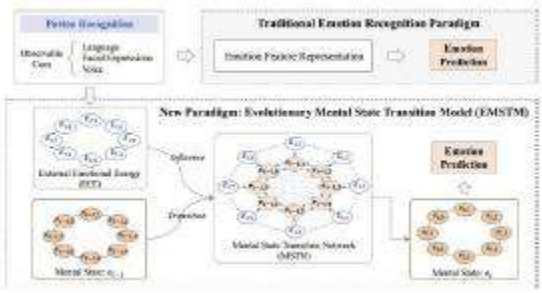

Fig. 1. High-level overview of EMSTM. Multi-modal features are fused into *external emotional energy* (EEE), which then drives hidden emotional states via MSTN

2. PROPOSED METHOD: EMSTM

A. *Multi-modal EEE Extraction*

We assume we have three modalities at time t: $x_{l,t}$ (lan- guage), $x_{v,t}$ (vision), and $x_{a,t}$ (acoustics). These features, possibly derived from pre-trained embeddings (e.g., RoBERTa for text [17], Facet for vision, COVAREP for acoustics [9]), are each projected to dimension d. Following prior multi-head attention frameworks [18], we apply cross-attention blocks to capture inter-modality interactions. For instance, one block might use $x_{v,t}$ as queries and $x_{l,t}$ as keys/values. Another block might fuse $x_{l,t}$ and $x_{a,t}$, etc. Figure 2 shows a schematic for text-vision cross-attention.

After stacking these cross-modality blocks, we *pool* (using average plus max) the resultant representation into $z_t \in \mathrm{R}^d$. A linear projection $W_e \in \mathrm{R}^{d \times n}$ produces:

$$E_t = z_t W_e \quad \in \mathrm{R}^n, \qquad (1)$$

where n denotes the number of emotion categories (6 for CMU-MOSEI, 8 for Ren-CECps). We regard E_t as *external emotional energy*: a purely *observable* descriptor of how strongly each emotion might be triggered at time t.

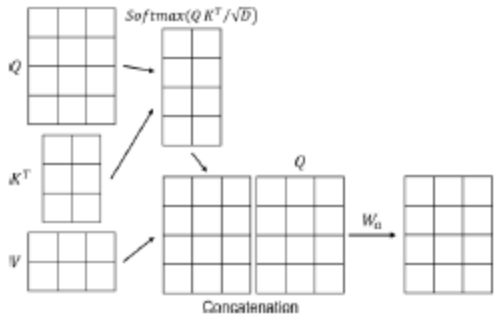

Fig. 2. Multi-head cross-attention mechanism to fuse textual and visual cues. We stack additional blocks for acoustic data, then pool results.

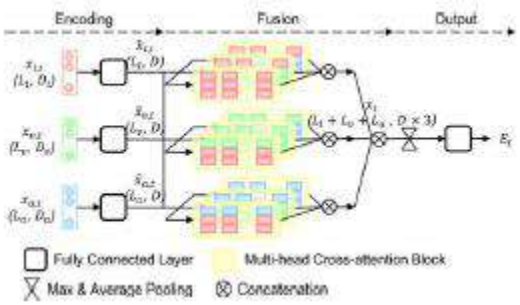

Fig. 3. Detailed pipeline for multi-modal EEE extraction. Each modality is projected to a unified dimension; we optionally pad or mask sequences with different lengths. Then, multiple cross-attention blocks fuse signals from text, vision, and acoustics. Finally, we aggregate with both average and max pooling to form z_t, which is projected into $E_t \in \mathrm{R}^n$

Figure 3 further illustrates how these modalities can have varying sequence lengths or feature dimensions. We align them (via projection or zero-padding) and pass them into multiple cross-attention layers. After these layers highlight critical interactions (e.g., linking a spoken phrase to a specific facial expression), we pool to form z_t, capturing both focal and background information. Finally, we map z_t to E_t, distributing energy across n emotions. Notably, E_t is *not* a direct label distribution but an *external* driver that may shift deeper emotional states.

B. *Mental State Transition Network (MSTN)*

While E_t approximates external signals, the *true* underlying emotion is modeled by $e_t \in \mathrm{R}^n$, each dimension $e_{t,i} \in [0, 1]$ reflecting intensity of emotion i. We maintain a 3D transition tensor $T \in \mathrm{R}^{n \times n \times n}$. The old state e_{t-1} transitions to e_t under the impact of E_t. Specifically,

$$\tilde{e}_{t-1} = \mathrm{Norm}\ E_t \times e_{t-1} \times T \quad , \qquad (2)$$

where ($e_{t-1} \times T$) redistributes intensities across possible emotion categories, modulated by E_t. We normalize to prevent numerical overflow or vanishing. Finally:

$$e_t = \text{Concat}\, \tilde{e}_{t-1}, E_t\, W_c, \qquad (3)$$

where $W_c \in \mathrm{R}^{2n \times n}$. If $e_{t,i} > \theta$, we label emotion i as present at time t. Unlike typical RNNs or transformers, MSTN focuses
on a compact n-dimensional state, referencing EEE each step to handle short-term influences.

C. *Training for Multi-Label Classification*

Real human affect can contain multiple simultaneous emotions (e.g., sadness and anger). Hence, $e_t \in \mathrm{R}^n$ is interpreted as n logits for time t. Let $Y_{t,i} \in \{0, 1\}$ be ground-truth presence of emotion i. We sum a margin-based loss, such as circle loss [19], over positive and negative categories:

$$L = \sum_{i=1}^{n} \mathbf{1}(Y_{t,i} = 1)\, \phi(e_{t,i}, +) + \mathbf{1}(Y_{t,i} = 0)\, \phi(e_{t,i}, -) \,. \qquad (4)$$

After training, we pick threshold(s) near zero for each emotion dimension, deciding if $e_{t,i}$ surpasses that boundary to label emotion i. EMSTM thus accommodates multi-label classification with sequential transitions, ensuring that historical states inform the current step.

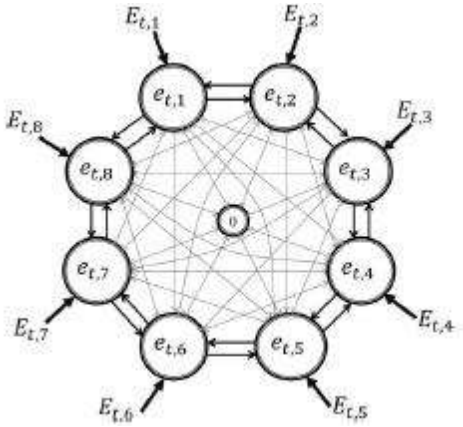

Fig. 4. Conceptual MSTN flow for $n = 3$ example. EEE shapes how intensities from e_{t-1} move into e_t, reflecting psychoanalytic ideas that observed signals partially drive deeper emotion.

3. Experiments and Results

We evaluate EMSTM on two multi-label emotion datasets: the multi-modal CMU-MOSEI and the monomodal Ren- CECps. Comparisons include classical multi-label approaches (BR, BP-MLL) and specialized neural architectures (G-MFN, Mu-Net). We train with AdamW [20] at a 1e-3 learning rate, batch size 64, and apply early stopping.

A. *CMU-MOSEI*

1) Dataset and Setup: CMU-MOSEI [9] consists of 23,453 labeled segments from monologues, annotated for six emotions: happiness, sadness, anger, disgust, fear, surprise.

We adopt the official train/test splits. GloVe or RoBERTa embeddings handle text, while Facet and COVAREP capture facial and acoustic features. This dataset displays notable imbalance, with happiness and sadness more frequent than fear or surprise.

2) Comparison with Baselines: Table I reports per-emotion accuracy (Acc), F1, and a weighted accuracy (WA). "W/OMSTN" classifies E_t directly, ignoring transitions. Incorporating MSTN (EMSTM) yields a ≈0.8% WA gain, especially for frequent classes. Using RoBERTa (EMSTM(L)) further boosts WA from 78.0% to 79.2%. Gains for minority labels (fear, surprise) are smaller but still evident, suggesting MSTN references prior states to refine predictions.

B. Ren-CECps

1) Dataset and Setup: Ren-CECps [10] is a text-based Chinese blog dataset of 27k training and 7.6k test samples, each annotated for eight emotions. We measure micro-F1, macro-F1, average precision (AP), coverage error (CE), and ranking loss (RL). Although single-modality, it tests MSTN's ability to capture transitions over consecutive textual snippets.

2) Performance: Table II shows that MSTN surpasses base- line approaches (BR, BP-MLL) and hierarchical/conv-based text models (HAN, DPCNN). Even a strong FC classifier with BERT is outperformed by MSTN's dynamic transitions, especially in macro-F1. Gains in micro-F1 and ranking-based metrics confirm that referencing prior states clarifies multi- label overlaps and intensities.

4. DISCUSSION

A. Parameter Efficiency for Real-Time Applications

In contrast to large sequential models that propagate multi- modal features step-by-step, MSTN updates only an *n*- dimensional state each step while referencing EEE. Figure 5 illustrates approximate parameter counts, revealing that EMSTM remains at around 0.59M parameters, considerably less than many multi-modal baselines. Such compactness is promising for real-time scenarios, from social robot interactions to mobile apps with constrained computational resources.

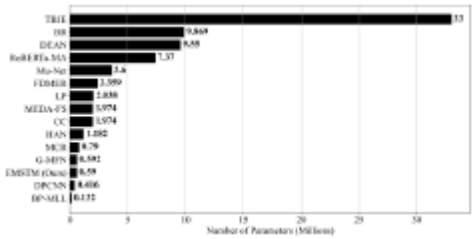

Fig. 5. Approximate parameter counts comparing EMSTM and baselines, demonstrating EMSTM's relatively small footprint.

B. Addressing Minority Emotions and Future Directions

Although MSTN improves performance for frequent classes, minority categories (e.g., fear, surprise in CMU- MOSEI) remain challenging. Future extensions might combine MSTN with data augmentation or weighting schemes to mitigate class imbalance.

Another approach is to adapt the transition tensor T to each user's personality [7], acknowledging individual differences in emotional reactivity. Expanding EEE to include additional modalities (e.g., EEG signals [21], GSR) could capture more subtle states. Lastly, we envision personalizing MSTN for repeated user interactions, exploring how persistent emotional styles influence transitions.

C. CONCLUSION

We presented an **Evolutionary Mental State Transition Model** (EMSTM) that explicitly differentiates *external emotional energy* (EEE) from deeper emotional states, linking them through a *mental state transition network* (MSTN). By fusing multi-modal signals into EEE and updating a compact latent state, EMSTM outperforms conventional methods on CMU-MOSEI and Ren-CECps while maintaining efficiency. Future work includes addressing minority emotion labels, expanding EEE with additional modalities, and personalizing transition tensors to each user. Our findings underscore that explicitly modeling transitions in hidden affect, rather than equating external signals with emotion, yields a more faithful and robust depiction of human affect dynamics.

Acknowledgments

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Research on 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, 2023).

Schaefer is the author of more than 1700 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 was held in Professor Schaefer's honor in December 2022 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 82 undergraduate researchers who have published papers with him, 138 successful Ph.D. students (plus 12 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 significant positions in industry (Accelrys, Adesis, ALTANA, Amazon Web Services, 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, General Dynamics Information Technology, 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, Nvidia, OpenEye, OSI Software, PartnerRe, Pfizer, Pharmaceutical Research Associates, Polaroid, Proctor & Gamble, Q-CHEM, Quantinuum, Raytheon, Reagens Deutschland, Ricoh, RWDC Bioplastics, Schroedinger, SciCo, Sugen, Susquehanna International Group, 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 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, University of California at Santa Cruz, City University of New York, University of Concepcion (Chile), Duke University, Emory University, Fatih University (Istanbul, Turkey), George Mason University, 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, Missouri Institute of Science and Technology, 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 Deputy Editor-in-Chief 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 was the sole recipient of the Gold Medal of the American Institute of Chemists. Seven of the previous 14 recipients of the AIC Gold Medal received the Nobel Prize. Most recently, 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 86,000 times. Professor Schaefer's Clarivate Web of Science H-index is currently 127. He has published 183 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.

Atomic Layer Deposition of ScF3 and ScxAlyFz Thin Films

by Markku Leskelä, Member EUAS

Short Biography

Markku Leskelä *(born 1950) received both M.Sc. (1974) and PhD (1980) degrees from Helsinki University of Technology. During 1979-1986 he worked at University of Oulu and Helsinki University of Technology as associate professor or acting professor, in 1986-1990 at University of Turku as professor and in 1990-2018 at University of Helsinki as professor of inorganic chemistry. He made sabbatical visits in 1983 (University of Utrecht), 1987-1988 (University of Florida) and in 1999 (University of Paris VI). During 2004-2009 he served as Academy professor. Since 2019 he has worked as emeritus professor at University of Helsinki.*

His research interests cover luminescent materials, catalytic activation of small molecules with metal compounds, and development of chemistry for Atomic Layer Deposition of thin films – the latter topic being dominating during last eight years. He has worked as vice-director (2002-2007) and director (2012-2017) in two centers of excellence funded by Academy of Finland. He has published about 740 original and 65 review papers which have been cited 58 800 times (h-index 117; Google Scholar). He holds more than 40 patents. He was nominated in 2004 as ISI Highly Cited Author in materials science. He has received several honors and awards: Magnus Ehrnrooth Foundation Award in Chemistry (2002), SVR I (2005), A.I. Virtanen award (2011), American Vacuum Society ALD innovation award (2012), Honorary award of Finnish Academy of Sciences and Letters (2014), Honorary member (2014) and honorary chairman (2019) of Finnish Chemical Society, Honorary doctor (University of Tartu 2016). He is a member of four academies of sciences. He has and has had several positions of trust in universities (for example board of trustees of University of Helsinki 2010-2017), scientific societies (for example IUPAC Div II, 2006-2017, secretary of the Division 2012-2017), academies (president of the Finnish Academy of Technical Sciences 2019-2022 and the chairman of The Council of Finnish Academies (CoFA) 2021-2022) foundations (for example Alfred Kordelin Foundation 2009-2017, chairman of the Foundation for Chemistry Congress 2013-2026).

E. Atosuo, M.J. Heikkilä, J. Majlund, L. Pesonen, M. Mäntymäki, K. Mizohata, M. Leskelä, M. Ritala: Atomic Layer Deposition of ScF_3 and $Sc_xAl_yF_z$ Thin Films. *ACS Omega* 2024, 9, 11747−11754.

In this paper, we present an ALD process for ScF_3 using $Sc(thd)_3$ and NH_4F as precursors. This is the first material made by ALD that has a negative thermal expansion over a wide-temperature range. Crystalline films were obtained at the deposition temperatures of 250−375 °C, with a growth per cycle (GPC) increasing along the deposition temperature from 0.16 to 0.23 Å. Saturation of the GPC with respect to precursor pulses and purges was studied at 300 °C. Saturation was achieved with $Sc(thd)_3$, whereas soft saturation was achieved with NH_4F. The thickness of the films grows linearly with the number of applied ALD cycles. The F/Sc ratio is 2.9:3.1 as measured by ToF-ERDA. The main impurity is hydrogen with a maximum content of 3.0 at %. Also carbon and oxygen impurities were found in the films with maximum contents of 0.5 and 1.6 at %. Nitrogen was not found in the films. The film morphology is lamellar type, especially at lower deposition temperatures, as investigated by FESEM. The films are rough; for example, for a 78 nm film deposited at 300 °C the Rq is 5.9 nm.

The ScF_3 process was also combined with an ALD AlF_3 process to deposit $Sc_xAl_yF_z$ films. In the AlF_3 process, $AlCl_3$ and NH_4F were used as precursors. It was possible to modify the thermal expansion properties of ScF_3 by Al^{3+} addition. The ScF_3 films shrink upon annealing, whereas the $Sc_xAl_yF_z$ films show thermal expansion, as measured with HTXRD. The thermal expansion becomes more pronounced as the Al content in the film is increased. It is thus possible to tune the thermal expansion properties of ScF_3 by the addition of Al^{3+} ions to the structure. It is assumed that by finding the right Sc/Al ratio, obtaining a zero thermal expansion material with ALD is possible.