EU ACADEMY OF SCIENCES

EUAS

EU ACADEMY
2017 ANNUAL REPORT

Board of Governors

President

Professor E.G. Ladopoulos (2000 Outstanding Scientists 20th-21st Centuries)

Governors

Board of Governors in the Division of Engineering and Physics:

Professor S. Glashow (Nobel Physics 1979)

Professor J. Friedman (Nobel Physics 1990)

Professor G. Smoot (Nobel Physics 2006)

Board of Governors in the Division of Chemistry:

Professor Y.T. Lee (Nobel Chemistry 1986)

Professor R. Ernst (Nobel Chemistry 1991)

Professor M.Levitt (Nobel Chemistry 2013).

Professor F. Stoddart (Nobel Chemistry 2016).

Board of Governors in the Division of Medicine:

Professor C. Greider (Nobel Medicine 2009)

Professor R. Schekman (Nobel Medicine 2013)

Professor S. Yamanaka (Nobel Medicine 2012).

Board of Governors in the Division of Social Sciences, Law & Economics:

Professor D. Kahneman (Nobel Economics 2002)

Professor P. Krugman (Nobel Economics 2008)

Professor J. Stiglitz (Nobel Economics 2001)

Professor E. S. Phelps (Nobel Economics 2006).

Contents

7 Maximum Speed of Light for the Future Spacecraft by Relativistic Elasticity, Thermo-Elasticity & Universal Mechanics Suitable for the Nobel prize ?
by Prof. Evangelos Ladopoulos, President & CEO of EUAS

12 Innovative & Groundbreaking Supramolecular Chemistry and Nanotechnology – Nobel Lecture.
by Prof. Sir Fraser Stoddart, Governor EUAS

18 Strategies for delivering Biotech Macromolecules: the Small Intestine, Cheek, and Joints.
by Prof. David J. Brayden, Member EUAS

22 Earthquake and Structural Engineering.
by Prof. Guiqing Li, Member EUAS

26 Digital Content Analytics and Computational Science.
by Prof. Fionn Murtagh, Member EUAS

29 Advanced Materials for Energy Storage & Conversion.
by Prof. Zongping Shao, Member EUAS

32 New Aspects in Cardiovascular Research & Echocardiography.
by Prof. Thomas F. Lüscher, Member EUAS

35 Contributions to Rheology and Polymer Processing.
by Prof. Avraam I. Isayev, Member EUAS

42 Biomedical Materials and Clinical Biochemistry.
by Prof. Pankaj Vadgama, Member EUAS

46 Contributions in Obesity Surgery.
by Prof. Christine Stroh, Member EUAS

50 Materials Science, Novel Materials for Energy Storage and Conversion.
by Prof. Meilin Liu, Member EUAS

54 New Contributions in Cardiovascular Medicine.
by Prof. Hiroaki Shimokawa, Member EUAS

58 innovative Aspects in Biochemistry.
by Prof. Etana Padan, Member EUAS

63 Robotics and New Energy System Research.
by Prof. Aarne Halme, Member EUAS

67 Innovative Methods in Airway Disease Research.
by Prof. Peter Barnes, Member EUAS

71 Biomimetic Physics: Learning from Evolutionary Strategies of Overcoming Evolutionary Crises. Nature as Material Designer.
by Prof. Erich Sackmann, Member EUAS

78 Nanoglasses: A Way of alloying Materials that are immiscible in all of Today's Materials?
by Prof. Herbert Gleiter, Member EUAS

82 Innovative Research in Plasticity Engineering.
by Prof. Michael Kassner, Member EUAS

86 Neutron Reflectivity of Spintronic Materials.
by Prof. Hartmut Zabel, Member EUAS

92 Game Theory-Based Control System Algorithms with Real-Time Reinforcement Learning.
by Prof. Frank Lewis, Member EUAS

96 Innovative Research in Alzheimer's Disease (AD).
by Prof. George Perry, Member EUAS

99 New Aspects of Experimental Physics of Interfaces.
by Prof. Hans-Jürgen Butt, Member EUAS

103 Quantum Dot Based Photonics:The Markets are now coming.
by Prof. Dieter H. Bimberg, Member EUAS

109 Fabric Formwork: A New Form of Architecture.
by Prof. Tim Ibell, Member EUAS

113 Innovative Aspects in Tribology, Fatigue & Damage Analysis.
by Prof. Michael Khonsari, Member EUAS

117 Advanced Technologies & Diagnostic Spin-Outs.
by Prof. Carl Borrebaeck, Member EUAS

121 Process Machinery & Systems Engineering.
by Prof. Eberhard Schlücker, Member EUAS

125 Developments in Wind Engineering.
by Prof. Qiu-Sheng Li, Member EUAS

129 Research in Optical Properties of Materials: Theory & Practice.
by Prof. David Aspnes, Member EUAS

131 Mechanical Properties of Lightweight Materials.
by Prof. Daolun Chen, Member EUAS

135 Appropriate Technology for Fighting Energy Poverty Developing Countries.
by Prof. Antonio Lecuona-Neumann, Member EUAS

139 Innovative Energy Research & Technology.
by Prof. Mohsen Assadi, Member EUAS

144 Structural Phenomenon of Concrete Elements at Limit States.
by Prof. Yuri Ribakov, Member EUAS

148 Innovative Improvements in Vascular Biology.
by Prof. Yihai Cao, Member EUAS

152 **Recent Developments in Materials Science of Metastable Materials.**
by Prof. Jürgen Eckert, Member EUAS

156 **Machine Learning and Optimization for Material Design Innovation.**
by Prof. Timon Rabczuk, Member EUAS

161 **The Essence of Importance Measures.**
by Prof. Way Kuo, Member EUAS

163 **Materials and Process Modelling Technologies.**
by Prof. Jianguo Lin, Member EUAS

168 **New Aspects for Development of Green Cements and Sustainable Infrastructure.**
by Prof. Paulo Monteiro, Member EUAS

172 **Solutions for Century Old Engineering Problems.**
by Prof. William Gerberich, Member EUAS

177 **Overview on Important Research Contributions in Polymer Opto-Electronics.**
by Prof. Show-An Chen, Member EUAS

181 **Can we create an Intelligent and Evolutionary Robot with a Brain?.**
by Prof. Fuji Ren, Member EUAS

185 **Contributions to Evolvable Assembly Systems.**
by Prof. Mauro Onori, Member EUAS

192 **Two Themes in Holomorphic Dynamics.**
by Prof. Mikhail Lyubich, Member EUAS

196 **Interaction between the Plasma Atmosphere of the Sun and its Magnetic Field.**
by Prof. Eric Priest, Member EUAS

200 **Recent Contributions in Applied Medicine.**
by Prof. John Forrester, Member EUAS

205 **Functional Organic- Inorganic Nanohybrid Materials.**
by Prof. Chang-Sik Ha, Member EUAS

210 **Motivation, Scope and Structure of the 2nd Edition of the Encyclopedia of Computational Mechanics with special Focus on the first two Volumes: Fundamentals.**
by Prof. Erwin Stein, Member EUAS

215 **Chemical Reaction Dynamics: Recent Advances and New Insights.**
by Prof. Kopin Liu, Member EUAS

219 **Recent Trends in Natural Gas Supply Chain Optimization.**
by Prof. Zuo-Jun Max Shen, Member EUAS

222 **Fatigue Crack Growth Behaviour of Steels in High Pressure Hydrogen.**
by Prof. Ashok Saxena, Member EUAS

227 **Overview on CBS Extrapolation and its Implications.**
by Prof. Antonio Varandas, Member EUAS

Maximum Speed of Light for the Future Spacecraft by Relativistic Elasticity, Thermo-Elasticity & Universal Mechanics Suitable for the Nobel prize ?

by Evangelos Ladopoulos, President & CEO of EUAS

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

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

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

Intensity Factors". Thus, the *"Universal Equation of Elasticity"*, the *"Universal Equation of Thermo-Elasticity"* and the *"Universal Stress Intensity Factors"* are parts of the general theory of *"Universal Mechanics"*.

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

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

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

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

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

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

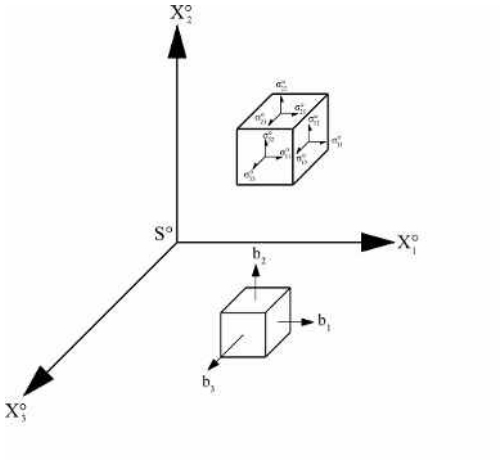


Fig. 1 The state of stress σ_{ik}^{0} in the stationary system S^{0}.

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

Hence, 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 $\mathbf{n}$:

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

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).

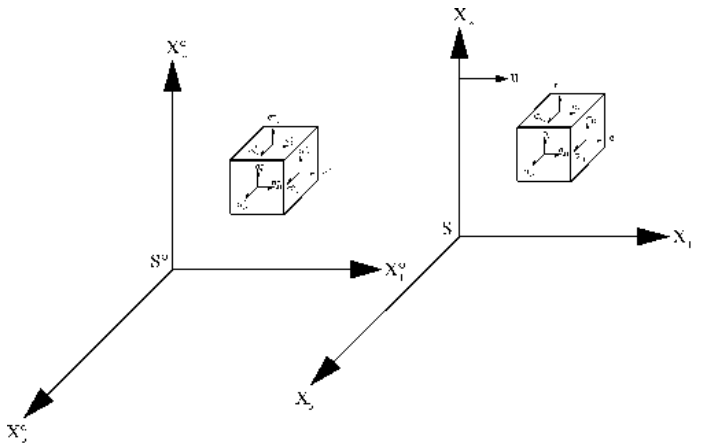


Fig. 2 The state of stress σ_{ik}^{0} in the stationary system S^{0} and σ_{ik} in the airframe system with velocity u parallel to the x_1 - axis.

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

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

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

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

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

where γ is given by:

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

with c the speed of light.

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

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

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

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

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

Thus, *"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. So, by the current author is completed the theory of Albert Einstein for the whole universe regarding mechanics engineering behavior.

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

Table 1

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

From Table 1 follows that for small velocities 50,000 *km/h* to 200,000 *km/h*, the absolute and the relative stress tensors are nearly the same. On the other hand, for bigger velocities like $c/3$, $c/2$ or $3c/4$ (c = speed of light), the variable γ takes values more than the unit and thus, relative stress tensor is very different from the absolute one. 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. Thus, as was shown by the current author, the relative first and third mode stress intensity factors are the same for both stationary and moving frames, while the relative second mode stress intensity factor is much different in the above frames. All the relative stress intensity factors (first, second and third) are important for the fracture mechanics analysis of the future spacecraft, as for their fracture mechanics analysis a combination of all the three intensity factors should be used.

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

Innovative & Groundbreaking Supramolecular Chemistry and Nanotechnology Nobel Lecture

by Sir Fraser Stoddart, Governor EUAS

Short Biography

The academic career of Fraser Stoddart, who was born in the capital of Scotland on Victoria Day (May 24) in 1942, can be traced through thick and thin from the Athens of the North to the Windy City beside Lake Michigan with interludes on the edge of the Canadian Shield beside Lake Ontario, in the Socialist Republic of South Yorkshire, on the Plains of Cheshire beside the Wirral, in the Midlands in the Heartland of Albion, and in the City of Angels alongside the Peaceful Sea. He was raised, an only child, on a mixed-arable farm a dozen miles south of Edinburgh. His formal education began with his attending the local village school in Carrington, Midlothian when he was four. A rigorous introduction to the three Rs – namely, reading, writing and arithmetic – made it relatively easy for him to make the transition to Melville College, a high school in the middle of Edinburgh. He went to Edinburgh University in 1960 and graduated with a BSc degree in 1964. During his time as a postgraduate student in the Department of Chemistry he cut his teeth in research investigating the nature of plant gums of the Acacia genus within the School of Carbohydrate Chemistry under Professor Sir Edmund Hirst.

In March 1967, Stoddart took his leave of the Chemistry Department at Edinburgh with a PhD degree to spend the next three years as a National Research Council of Canada Postdoctoral Fellow at Queen's University with Professor J. K. N. Jones. No sooner had he arrived in Kingston, Ontario than a communication appeared in the Journal of the American Chemical Society by Charles Pedersen (one of three Nobel Laureates in Chemistry in 1987) describing the synthesis of dibenzo[18]crown-6 in excellent yield as a consequence of the templating action of potassium ions. This seminal event marked the beginning of Fraser's fascination with chemistry beyond the molecule, which, combined with his interest in templation, has led to the template-directed synthesis, based on molecular recognition and self-assembly processes, of a wide range of mechanically interlocked molecules (e.g., catenanes and rotaxanes), variants of which have found their way into molecular electronic devices, drug delivery systems, and molecular machines. Mechanically interlocked molecules – or MIMs for short – are discussed at length in "The Nature of the Mechanical Bond : From Molecules to Machines" written in conjunction with ex-graduate student, Carson Bruns, and published by Wiley in November 2016.

Fraser met Edinburgh graduate Norma Scholan (BSc chemist/PhD biochemist) in 1966 while he was a postgraduate student in the Chemistry Department at Edinburgh and they started their married lives in Canada in 1968. In 1970, they returned to the United Kingdom so that Fraser could take up an Imperial Chemical Industries (ICI) Fellowship at Sheffield University where he worked briefly with Professor W. D. Ollis before being appointed as a Lecturer in Chemistry. After spending a three-year sabbatical (1978–1981) at the ICI Corporate Laboratory in Runcorn, he returned to Sheffield where he was

promoted to a Readership in Chemistry. It was during his time at ICI that Stoddart developed his long-standing interest in bipyridinium units (constituents of the ICI herbicides Diquat and Paraquat) as redox-addressable building blocks for incorporation into bistable catenanes and rotaxanes. On 23 May 2013, Fraser published his 1000th scientific paper: the total count has now reached 1120. He has trained >450 graduate and postdoctoral students of which >100 have subsequently embarked on successful independent academic careers.

In 1990, he took up the Chair of Organic Chemistry at Birmingham University where he was Head of the School of Chemistry (1993–97) before moving to the University of California, Los Angeles (UCLA) as the Saul Winstein Professor of Chemistry in 1997. In 2002, Fraser became the Director of the California NanoSystems Institute (CNSI) and assumed the Fred Kavli Chair of NanoSystems Sciences. He joined the faculty at Northwestern University in 2008 as a Board of Trustees Professor of Chemistry and was Director of the Center for the Chemistry of Integrated Systems (CCIS) from 2010 to 2017.

In 2014, he became the Chief Technical Officer at PanaceaNano and at Cycladex, as well as being a Thousand Talent Scholar at Tianjin University in China. In 2018, he will become a Part-Time Professor of Chemistry at the University of New South Wales in Sydney, Australia.

Fraser is a Fellow of the Royal Society of London, the German Academy (Leopoldina) of Natural Sciences, and the Royal Netherlands Academy of Arts and Sciences, as well as an Honorary Fellow of the Royal Society of Edinburgh and the Royal Society of Chemistry. He is a Member of the American Academy of Arts and Sciences, the National Academy of Sciences, and the EU Academy of Sciences. He is a Foreign Member of the Chinese Academy of Sciences.

Stoddart was appointed by Her Majesty Queen Elizabeth II as a Knight Bachelor in her 2007 New Year's Honours List for services to chemistry and molecular nanotechnology. In this same year, he won the King Faisal International Prize in Science. In 2010, he was the recipient of a Royal Medal, granted by Her Majesty Queen Elizabeth II and presented by Prince Philip, Duke of Edinburgh. He was awarded the Nobel Prize in Chemistry in 2016 for his design and synthesis of molecular machines.

Fraser's and Norma's daughters, Fiona (b. 1973) and Alison (b. 1976), are both PhD chemists! In 2004, Norma succumbed to a 12-year battle with breast cancer. Fiona lives with her Australian husband and their two children in Belmont, MA while Alison, who is the Editor of Nature Reviews Materials, lives in Cambridge, UK with her Chinese husband and their three sons. To learn more about the life and works of ***Fraser Stoddart****, read about "Big and Little Meccano" in Tetrahedron* ***2008****, 64, 8231–8263 and Mechanically Interlocked Molecules (MIMs) – Molecular Shuttles, Switches and Machines (Nobel Lecture) in the International Edition of Angewandte Chemie* ***2017****, 56, 11094–11125.*

Sir Fraser Stoddart

The 'post-truth' era of fake news is nothing new, it seems. It has long been claimed in the media that Prince Charles warned that self-replicating nanobots could turn the world into 'grey goo' – a phrase he denies using. In fact, the Prince was merely quoting a

warning from nanoscientist Dr Eric Drexler, who later walked back such claims. Prince Charles did say that new technology had to be used "wisely and appropriately" and lauded nanotechnology as a "triumph of human ingenuity", saying that "some of the work may have fundamental benefits to society, such as enabling the construction of much cheaper fuel-cells, or new ways of combating ill-health."

The science-fiction apocalyptic image is far from the truth, but understandable, given the incredible ingenuity involved in creating miniature mechanical devices at an atomic scale. In fact, it wasn't until 1981, with the development of the scanning tunneling microscope that can let us 'see' individual atoms, that modern nanotechnology became possible. The 2016 Nobel Prize in Chemistry rewarded three pioneers in the field – Jean-Pierre Sauvage**,** Sir Fraser Stoddart and Ben Feringa – for their design and production of molecular machines which can perform controlled tasks when energy is supplied.

Frenchman Sauvage set the wheels in motion, quite literally, by coming up with a means of producing molecules called catenanes in which two or more rings are linked together mechanically to form a chain. These molecules have served as prototypes of rotary motors.

The next step was taken by Fraser Stoddart, who produced the blueprint for linear molecular motors, in the shape of mechanically interlocked molecules called rotaxanes, in which a ring trapped on the axle of a dumbbell is capable of controlled movement back and forth along the axle of the dumbbell. These molecular shuttles were the forerunners of molecular switches, which were incorporated into molecule-based computer chips and, as nanovalves, into drug delivery systems. Subsequently, the molecular switches have been integrated into molecular machines, such as molecular muscles and artificial pumps.

Sir Fraser performed much of his work at University of California, Los Angeles (UCLA) where his team produced large-scale 'ultra-dense' memory devices that store information using controllable molecular switches. This research represented an important step toward the creation of molecular computers that are much smaller and potentially more powerful than today's silicon-based counterparts. Stoddart himself said: "This research was the culmination of a long-standing dream that these molecules could be used for information storage."

He also developed mechanically interlocked molecules called suitanes, named for their appearance like a limbed torso in a suit. "Discovering the way to dress a molecule with another one is a prelude to constructing artificial systems reminiscent of living cells", said Stoddart.

Fraser Stoddart was born in Edinburgh, Scotland, in May 1942, and grew up on a farm near Carrington, Midlothian, where he attended the local school before going on to Melville College in Edinburgh. At the University of Edinburgh he earned his BSc in 1964 and PhD in 1966, after which he went to Queen's University in Kingston, Canada as a postdoctoral fellow, returning to the United Kingdom in 1970 as a research fellow at the University of Sheffield. He stayed on there as a lecturer, and later as a reader in chemistry, while working as a visiting research fellow at UCLA and spending three insightful years (1978-81) on secondment to the ICI Corporate Laboratory in Runcorn, Cheshire. During this time he was awarded a DSc degree (1980) by the University of Edinburgh for his

research into stereochemistry beyond the molecule. In 1990 he became chair of organic chemistry at the University of Birmingham, and in 1997 moved to UCLA to become the Winstein Professor of Chemistry in 1997. In 2002, he joined the California NanoSystems Institute as the Kavli Professor of Nanoscience, rising to director before, in 2008, joining Northwestern University as a Board of Trustees Professor and establishing a Mechanostereochemistry Group in Evanston, Illinois.

Sir Fraser is a Fellow of the Royal Society of London, the German Academy (Leopoldina) of Natural Sciences, and the Royal Netherlands Academy of Arts and Sciences, as well as an Honorary Fellow of the Royal Society of Edinburgh and the Royal Society of Chemistry. He is a Member of the American Academy of Arts and Sciences, the National Academy of Sciences, and the EU Academy of Sciences. He is a Foreign Member of the Chinese Academy of Sciences.

Stoddart's awards include, in 2007, the King Faisal International Prize in Science and the Albert Einstein World Award of Science. He was appointed a Knight Bachelor in 2007. In 1968, he married fellow Scottish chemist Norma Scholan, who later worked with him and with whom he has two children; his daughter Alison is also a chemist and Chief Editor of the journal, *Nature Reviews Materials*. After Norma's death in 2004, the family set up an annual award in her name for Academic Excellence and Outstanding Citizenship at UCLA.

Royal Society Research Professor David Leigh, one of many scientists trained by Stoddart, paid tribute to him, saying: "The credit for making molecular machines attractive to chemists goes to Fraser Stoddart. He had the vision to realise that these architectures gave you the possibility of large amplitude-controlled motions, and that that could be the basis of molecular machines."

Mechanically Interlocked Molecules (MIMs) – Molecular Shuttles, Switches, and Machines (Nobel Lecture)

Molecular Machines

A fundamental property of biological molecular machines, e.g., the motor proteins, is that they consume energy and drive systems away from equilibrium by controlling kinetic barriers. The emergence of the science of artificial molecular machines (AMMs) in the hands of chemists, for the most part, presents us with a steep learning curve to negotiate. Nonetheless, it is a challenge that the chemistry community has embraced increasingly during the past two decades with much of the teaching of the fundamental theory coming from the physics community, and, in particular, one very prominent physicist from the University of Maine, namely Dean Astumian with whom we have collaborated as well as published several reviews that stand alongside a crop that can be traced back for at least two decades from the present day. In my Nobel Lecture, I chose to highlight the progress we have made in recent times on the design and synthesis of artificial molecular pumps, based on the building blocks that found their origins almost 40 years ago in the ICI Corporate Laboratory and were used by us to put the mechanical bond on a firm footing before introducing them into molecular switches in the first instance.

Unidirectional Transport

At the outset, we designed and synthesized a constitutionally unsymmetrical dumbbell and demonstrated that it transports the **CBPQT^{4+}** ring in a unidirectional manner. In its midriff, the dumbbell houses an electron rich 1,5-dioxynaphthalene (DNP) unit which is capable of recognizing the electron poor **CBPQT^{4+}** ring. Kinetic control of the threading and dethreading of the dumbbell by the ring is managed by arranging to have a neutral isopropylphenyl (IPP) unit at one end of the dumbbell and a positively charged 3,5-dimethylpyridinium (PY$^+$) unit at the other end. The **CBPQT^{4+}** ring finds its most thermodynamically stable location on the DNP unit by passing over the IPP unit for the simple reason that the positively charged ring is repelled by the PY$^+$ unit. When the **CBPQT^{4+}** ring is reduced to **CBPQT$^{2(\bullet+)}$**, the relative heights of the two barriers change on account of the significantly decreased Coulombic barrier confronted by the ring which also, most likely, undergoes a reduction in size, resulting in increasing steric interactions with the PY$^+$ unit. At the same time, the donor–acceptor interactions between the **CBPQT$^{2(\bullet+)}$** ring and the DNP recognition unit are nullified, resulting in a preference for the rings to dethread into solution over the charged end of the dumbbell. In what is essentially a supramolecular system, no work is done: rings are extracted out of solution onto the dumbbell momentarily before being released back into solution.

Radical Interactions and Templation

Our initial approach to introducing unidirectionality into a supramolecular system employing donor–acceptor interactions demonstrated that we can control the relative motion between a dumbbell and a ring. The system, however, lacks the potential for it to be developed into a more sophisticated molecular machine where useful work can be done since the free energy change during the redox cycle is simply too small to be useful in a practical context. A discovery made in my research laboratory in 2010 by Ali Trabolsi and Albert Fahrenbach was to come to the rescue. They showed that a relatively strong tricationic trisradical complex (K_a = 10^4–10^5 M^{-1} in MeCN) is formed between **CBPQT$^{2(\bullet+)}$** and bipyridinium (**BIPY$^{\bullet+}$**) radical cations under reducing conditions. The strong binding affinity (attraction) can be switched back to being highly repulsive, following oxidation of the radical cations, in both instances, to give **CBPQT^{4+}** and **BIPY^{2+}**, resulting in a massive enthalpy change, something which struck us as being highly promising when it comes to designing and synthesizing AMMs to perform useful work.

We reasoned that we could achieve much better and more efficient unidirectional transport of **CBPQT^{4+}** rings if we were to replace the DNP unit in the constitutionally unsymmetrical dumbbell with a **BIPY^{2+}** unit and employ radical chemistry to form a stable rotaxane-like tricationic trisradical on reduction of both the ring and the **BIPY^{2+}** unit. We had already employed radical templation to synthesize a rotaxane – as well as a homo catenane – and demonstrated the strong repulsion that comes into play when the ring and recognition unit are oxidized back to CBPQT^{4+} and BIPY^{2+}, respectively.

Artificial Molecular Pump

Based on all these previous observations, and a large number of exploratory experiments conducted painstakingly by Chuyang Cheng, he settled on the design of an artificial molecular pump – call it Mark I – where an oligomethylene chain terminated by a stopper is attached at its other end to an IPP speed bump so that this portion of the dumbbell can act as a collecting chain for the rings transported from solution. In the oxidized state, the **CBPQT$^{2(\bullet+)}$** ring and the molecular pump portion of the dumbbell repel each other. Upon reduction, the **CBPQT$^{2(\bullet+)}$** ring passes quickly over the PY$^+$ unit in search of the radical recognition site, namely a BIPY$^{\bullet+}$ unit, to form the thermodynamically

favored trisradical tricationic complex. On oxidation, this complex becomes a highly unstable species carrying six positive charges. Under these circumstances, the $CBPQT^{4+}$ ring would like to relax to a more favored location. Although its returning to the bulk solution is thermodynamically favored, this pathway is blocked kinetically by the PY^{+} unit, which acts as a Coulombic barrier to deslipping of the ring. Hence, with the aid of thermal energy the ring passes over the IPP speed bump onto the collecting chain. When a second reduction is performed, the IPP unit prevents the association of the trapped ring with the **BIPY**$^{\bullet+}$ recognition site, enabling this site to attract a second **CBPQT**$^{2(\bullet+)}$ ring from solution. In this AMM two positively charged rings are collected by a positively charged dumbbell, reflecting a process that is neither entropically nor enthapically favored. Work is done! The artificial molecular pump operates away from equilibrium by relying on the consumption of redox chemical energy. Our findings have shown that the kinetics associated with two cycles are the same to all intents and purposes, suggesting that that the first ring to be trapped does not have a significant influence on the threading of the second ring. These results are promising since they indicate that it is possible to extend the two-cycle system into a multi-cycle one, opening up the possibility of synthesizing slide-ring materials. A couple of design modifications to the artificial molecular pump are being explored currently: one is to speed up the action of the pump in a Mark II version at least four-fold from two hours per redox cycle to 30 minutes and the other is to double the addition of rings to polymer chains by locating pumps at both ends of the chains.

Epilogue

In summary, our interest in AMMs was given a considerable fillip in 1991 with the advent of the molecular shuttle, and the demonstration of the first donor–acceptor bistable switch in 1994. During the past couple of decades, there have been many investigations carried out in collaboration with Vincenzo Balzani at the University of Bologna. Our entry into radical chemistry and radical templation in 2010 set the stage for going forward from entropically driven unidirectional translation with donor–acceptor systems under thermodynamic control in 2013 to enthalpically driven unidirectional transport in 2015 under kinetic control and continuing up to the present time.

In a recent Tutorial Review in *Chemical Society Reviews* on *Mastering the Non-Equilibrium Assembly and Operation of Molecular Machines*, we focus on the thermodynamics of AMMs and discuss how theory can influence the design principles for constructing molecular machines going forward. A lot of fundamental work remains to be done. It is too early to speak in an authoritative and informed manner about what will be the killer applications of AMMs. We are at the very early stages of knowing how to build them let alone use them. Let me use the analogy of manned flight, particularly in relation to where aviation had reached in 1927, the year in which Charles Lindbergh crossed the Atlantic Ocean in the Spirit of St Louis. An account of the practice of manned flight in 1927 is told in all its amazing glory and gory detail in *One Summer* by Bill Bryson. Compare and contrast the situation for aviation in 1927 with where it stands today as a form of mass transport that has, not only opened up country-wide travel, but has also brought Continents together on the grandest of scales. As far as MIMs and AMMs are concerned, they await the engagement of the next generation of chemists eager to exploit the nature of the mechanical bond in chemistry, while taking up the task of designing and synthesizing MIMs and putting them to good use. Insofar as the template-directed protocols have established themselves as the most efficient ways to make 'intelligent' MIMs, a breakdown of the recent literature, based on a random selection of 500 articles on catenanes and rotaxanes, has led to the visualization of the data in a pie chart. Presently, solvophobic, hydrogen bonding, donor–acceptor, and metal templation account for a good three-quarters of the chemical literature on the mechanical bond. There is every reason to believe that the rapidly accelerating, widespread interest in the chemistry of the mechanical bond, which only started to grow in a linear fashion year-by-year in 1990, is all set now to experience an era of exponential growth.

Strategies for delivering Biotech Macromolecules: the Small Intestine, Cheek, and Joints

by David J. Brayden, Member EUAS

Short Biography

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

Education

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

Employment

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

Honours/Awards

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

2014-	*Reappointed to Editorial Advisory Board of Advanced Drug Delivery Reviews*
2015	*Distinguished service award from the CRS Annual Meeting Programme Committee 2015*
	Appointed Adjunct Professor at National University of Ireland, Galway
2016	*Chairman of the Novo-Nordisk Foundation Challenge Programme on "oral drug delivery of biopharmaceuticals"*
2017	*Recipient of Marquis Who's Who® Albert Nelson Lifetime Achievement Award*
2017	*Appointed Senior Associate Editor "Therapeutic Delivery"*
2017	*Lead organiser for the first Keystone Conference on drug delivery (Dublin, 2019)*

David Brayden is a pharmacologist who studies the interaction of drugs with epithelia in order to help design drug dosage forms that cross barriers to reach their target. He began his career in 1985 with his PhD studying how ions flow across intestinal and sweat gland epithelia, as this is the key to the ion chloride transport defect in cystic fibrosis (CF). This work was continued during his postdoctoral fellowship at Stanford, CA, USA, a period when the gene for CF was discovered and the pathways of electrogenic sodium reabsorption and chloride secretion across various epithelial surfaces were elucidated. In 1991, he saw an opportunity to apply many of the epithelial bioassays he has used for ion transport to drug delivery and moved back to Ireland to join Elan Corporation. This was a period of unprecedented growth for the drug delivery industry and Elan became the 2nd largest drug delivery company in the World. In 10 years at Elan, he set up their *in vitro* pharmacology laboratory and became a project manager of several of Elan's Joint Ventures with US Biotech companies. Much of the research he worked on was into how to convert injectable peptides to oral forms, the creation of transdermal vaccines, using Peyer's patch M cells for oral vaccine targeting, and research with Elan's pioneering (and ultimately failed) efforts at the time into its Alzheimer's disease vaccine programme. In 2001, Brayden moved to University College Dublin's (UCD) veterinary school, ostensibly to teach veterinary pharmacology and also to teach drug discovery and development to its biologists. At UCD, he brought in grants from Science Foundation Ireland (SFI) in the area of using PEGylated polymers to deliver oral peptides, and from the EU FP7 programme to develop nanotechnology to orally deliver insulin and Glucagon-like Peptide 1 (GLP-1).

Brayden's current research is focussed on how to incorporate intestinal permeation enhancers into solid dosage forms to enable oral delivery of macromolecules and he has published extensively in the area [1]. He has collaborations with industry, including Sigmoid Pharma (2009-17), Merrion Pharmaceuticals (2010-14, Novo-Nordisk (2009-12), and Jazz Pharmaceuticals (2016-). Other strengths of the Brayden lab are in developing printed dissolvable films that can be attached to the cheek (buccal epithelium) in order to promote delivery of GLP-1 analogues. This work is part of his role as co-lead PI in the SFI Centre for Medical Devices (2014-2021), which is a national consortium with strong links to the Medical Device industry. Another project is in the area of intra-articular injection of nanoparticles in mice to offset joint inflammation [2], work that has moved on recently to the scale-up and testing of the hyaluronic acid based calcitonin "nano" system in an equine joint lipopolysaccharide model. He also works with food-derived peptide bioactives on other grants and has a new set of peptides to work with to devise oral dosage forms, in addition to those sourced from Pharma industry. The following [1]-[6] are a selection of his most important papers, along with a commentary for each on their impact.

Selected Publications and their citations (Google Scholar®):

1. Aguirre TA, Teijeiro-Osorio D, Rosa M, Coulter IS, Alonso MJ, & Brayden DJ. (2016). Current status of selected oral peptide technologies in advanced preclinical development

and in clinical trials. Adv.Drug Deliv. Rev. 106: 223-241. Impact Factor: 15.6. Citat.:33

A recent review from the top ranked review journal in Pharmaceutical Sciences. It was a collaboration between the partners in the European Union FP7 programme, TRANS-INT, which is investigation oral peptide delivery using nanoparticles. Brayden co-edited the Special Issue of ADDR and this review in which he was the corresponding author will likely be heavily cited as it assessed most of the clinical data with oral peptides that is currently in the public domain.

2. Ryan, S. M., McMorrow, J., Umerska, A., Patel, H. B., Kornerup, K. N., Tajber, L., Murphy, E. P., Perretti, M., Corrigan, O. I., & & Brayden, D. J.(2013). An intra-articular salmon calcitonin-based nanocomplex reduces experimental inflammatory arthritis. J. Controlled Release 167: 120-129. Impact Factor: 7.4; Citations: 40

From JCR the highest ranked journal in the delivery field, this paper resulting from four years of work showed that a nanocomplex of calcitonin and hyaluronic acid reduced expression of a set of inflammatory markers in activated macrophage and neutrophil cell lines. The team then tested the complex as a one-time intra-articular injection in the acute KBxN mouse model of inflammatory arthritis and showed reduction of the cartilage inflammatory markers and conferred efficacy similar to a steroid injection. The model was so difficult to use that this study may never be able to be repeated. Brayden assembled the team from three institutions to do these studies and this nanocomplex is now being tested in an equine model of arthritis.

3. Gullberg, E, Leonard M, Karlsson J, Hopkins AM, Brayden D, Baird, AW, Artursson, P (2001) Expression of specific markers and particle transport in a new human intestinal M-cell model.. Biochemical and biophysical Research Communications 279 (3), 808-881. Impact Factor: 2.5; Citations: 201.

A collaboration between UCD and Uppsala University led to the development of an in vitro M-like cell model where Caco-2 cells were co-cultured with Raji B lymphocytes and expressed features of Peyer's patches for oral vaccines. Several elements came together, the first time all-human cells had been used in such a design and the fact that the Caco-2 and Raji B cells were in separate compartments such that gene expression could be done in order to discover apical membrane receptors for oral vaccine targeting. In 2017, Brayden co-authored a Nature Protocol with some of the same group and with Louvain University researchers in which all the models were critiqued.

4. Ryan, S.M., Mantovani, G., Wang, X., Haddleton, D.M. & Brayden, D. J. (2008). Advances in PEGylation of important biotech molecules. Exp. Op. Drug Delivery 5 (4): 371-383. Impact Factor: 5.4; Citations: 278

This review on PEGylated peptides and proteins is one of the most cited papers in Exp. Opinion on Drug Delivery. It combines the knowledge from the polymer chemistry group at Warwick University, UK, with the biological sciences expertise of Brayden's group at UCD. It includes unique structures of the team's Science Foundation Ireland's-funded project (with Brayden as PI) on comb-shaped PEG methacrylate polymers conjugated to calcitonin that increased the half-life of the injected peptide without compromising efficacy in rats.

5. McClean, S. Prosser, E., Meehan, E., O'Malley, D., Clark, N., Ramtoola, Z., & Brayden, D.J. (1998). Binding and uptake of biodegradable poly-DL-lactide micro- and nanoparticles in intestinal epithelia. Eur. J. Pharmaceutical. Sci. 6, 153-163. Impact Factor: 3.8; Citations: 259

This work is now 20 years old, but is still being cited. It is an enduring paper from Brayden's career at Elan Pharma on examining PLG particle uptake in the gut. At the time it was a technical advance to use of microscopy and quantitation of particles in tissue. Its conclusion on optimum PLG particle diameters for uptake influenced formulation in particle design for the oral vaccine field. At the time, the authors had no idea that it would be so heavily cited. Perhaps it is because some disagreed with its findings!

6. Brayden, D.J., Creed, E.M., O'Connell, A., Leipold, H., Agarwal, R., & Leone-Bay, A. (1997). Heparin absorption across the intestine: effects of SNAC in rat in situ instillations and in Caco-2 monolayers. Pharm. Res. 14 (12), 1772-1779. Impact Factor: 3.3; Citat.: 91.

This was one of the first biological assessments of the Emisphere oral delivery technology, where the effect of the delivery agent, SNAC, was tested in in vitro and in vivo bioassays set up at Elan by Brayden. SNAC is now very much back in vogue as it is in Phase III trials for oral delivery of Novo-Nordisk's glucagon-like Peptide 1 (GLP-1) long acting analogue, semaglutide. Brayden's team at Elan worked with a parallel team at Emisphere to show that SNAC did not affect intestinal epithelial tight junctions, that it was working via a transcellular action, and that it could deliver a macromolecule in vivo. The impact of the paper contributed to later toxicology work in which SNAC effects on internal organs was assessed and viewed as being negligible.

Earthquake and Structural Engineering

by Guiqing Li, Member EUAS

Short Biography

Prof. Li graduated from civil engineering department of Hunan University of China in 1953. He was a postgraduate student studied structural dynamics in Harbin University of Technology in the period from 1959 to 1963. He was a Director, International Association of Structural Reliability and Safety; Director, China Association for Disaster Prevention; Vice Chairman, Council of Wuhan University of Technology (WUT); Vice Chairman, Society of Sciences and Technology, WUT; Vice Chairman, Academic Committee, WUT; Director, Institute of Aseismic Engineering Structures, WUT, which is changed to Wuhan University of Sciences and Technology. The main research interests and technical expertise are in wind engineering, earthquake engineering, structural dynamics, vibrations and stability of structures, structural reliability, structural control, expert system for design of buildings and structures. His research in these fields has resulted over 500 journal papers and published 14 books. He got two national awards, two awards of the first class of the scientific and technological progress from the Ministry of Education of China, the first-class award of scientific and technological progress of Hubei province, and several second awards.

A. Earthquake Engineering

In order to establish design standard of a new type of assembly frame-light plate buildings, the supporting structure of which is rib floor-hollow column, the thick of floor is 3cm only. A lot of testing including plate with rib, joints and full-size structure and a building testing have been conducted. Fig. 1 is a full size three storey frame in the instant before its collapse. It is obtained from frame testing that:

1. The effective width of plate as the flange of beam is 140-160cm.
2. The entire property of the assembly floor is almost same as that of poured-in-place concrete floor.
3. The first crack and main cracks occurred at beams. Therefore, the rib floor-hollow column is a strong column and weak beam structural system. It is well known that this system is a good aseismic one.
4. Fig. 1 shows that the collapse of the testing frame is caused by destruction of the first storey. Therefore, the strength of columns of the first storey must be larger than the other ones.

Fig. 1. Deformation of the three storey frame at the instance before its collapse

A full size five storey building, the supporting structure of which is also rib floor-hollow column, was also tested. This testing is divided four stages. The first, second, third and fourth stage are the empty frame, empty frame with end wall plates, empty frame with all outside wall plates and the empty frame with all outside wall plates and inside enterclose and 70% live load, i.e., the fourth stage is a prototype building, respectively. The four stage tests show that the transverse stiffness in the second stage increases to 285% since the effect of end wall plates; the transverse stiffness increases to 224% since the effect of all inside enterclose. It is necessary to point out that the transverse stiffness is almost not increased since the effect of all outside longitudinal wall plates. The damping of empty frame is about 2%, and the effect of inside and outside wall plates makes damping to increase to 200%.

In order to determine earthquake response of structure, it is necessary to study earthquake ground motion which is assumed as:

$$\ddot{U}_0(t) = f(t)X(t) \tag{1}$$

in which $\ddot{U}_0(t)$ is the acceleration of earthquake ground motion; $X(t)$ is a stationary random function; $f(t)$ is a determination function.

According to records of earthquake ground motion, $f(t)$ may be selected as one of the following:

1. $f(t) = constant$, for stationary random process.

2. $f(t) = At^b(T_0 - t)^c$, for non-stationary random process, where

$$T_0 = t_0 + t_1, \qquad b = \gamma t_0, \qquad c = \gamma t_1, \qquad A = a_0\left(t_0^{t_0} t_1^{t_1}\right)^{-\gamma} \tag{2}$$

in which, a_0 is the maximum of standard deviation of acceleration of earthquake ground motion at $t = t_0$; T_0 is the duration of earthquake; γ is related to the variation of earthquake ground motion.

3. $f(t) = a_0\left(1 - \frac{t}{T_0}\right)^t e^{-ct}$, for decrease progressively non-stationary random process, (3)

in which, a_0 is the standard deviation of acceleration of earthquake ground motion at $t = t_0$; T_0 is the duration of earthquake ground motion; c is a decrease progressively factor. The earthquake response spectra were shown in the book [1].

B. Wind Engineering

The main contributions in wind engineering are as follows:

1. Maximum Wind Velocity Statistics

Wind velocity may be divided two parts: average and fluctuating wind velocity. Average wind velocity is a random variable, and fluctuating wind velocity is a random process. The statistical method of average wind velocity was proposed by Li [2] as follow:

$$t = C_1 + C_2 x + C_3 \log(x - k_0) \tag{4}$$

where x is the maximum average wind velocity; k_0 is the minimum of all maximum average wind velocities and obeys extremum distribution:

$$\Phi(t) = e^{-e^{-t}} \tag{5}$$

The procedure of statistic is as follows:

(1) Arrange all maximum average wind velocities in order from the largest to smallest, $x_1, x_2 \cdots x_m \cdots x_n$

(2) Calculating

$$P_m = P(x > x_m) = \frac{m}{n+1} \tag{6}$$

where n is the number of maximum average wind velocities.

(3) Solving the following equation gives t_m

$$P_m = \int_{t_m}^{\infty} e^{-e^{-t}} dt = 1 - \int_{-\infty}^{t_m} e^{-e^{-t}} dt \tag{7}$$

(4) K_o is the minimum in the range of maximum wind velocities, usually, it is taken zero.

(5) Determining C_1, C_2 and C_3 by using least-square method.

(6) Correlation function $K_x(\tau)$ and spectra of fluctuating wind velocity $S_x(\omega)$. It was proposed by Li [2] that

$$K_x(\tau) = e^{-\beta\tau}\left(\cos\gamma\tau - \frac{\beta}{\gamma}\sin\gamma|\tau|\right) \tag{8}$$

$$S_x(\omega) = b\frac{\omega^2}{\omega^2 + 2a_1\omega^2 + 2a_2^4} \tag{9}$$

According to the climate of south area of China, we found:

$$b = 9.67018\mathbf{k}V_{10}{}^2, \beta = \mathbf{1.90042}a, \gamma = \mathbf{1.6334}\alpha_1, a_1 = V_{10}\frac{\pi}{\mathbf{600}}, a_1 = \beta^2 - \gamma^2, a_2{}^2 = \beta^2 + \gamma^2$$

k --- coefficient of ground roughness; V_{10} --- velocity at the height 10m

C. Structural Control

Structural control is divided passive, active and semi-active control. Passive control is widely used in engineering because it is simple, economic and reliable, while active control is widely studied.

Our contributions are as following:

1. Riccarti equation is solved by use of decreasing power method.
2. Optimum locations of control forces
   (1) Criteria of optimum locations of control forces.
      (a) Optimum locations are based on the safety of a structure.
      (b) Optimum locations are based on the comfort requirements.

(2) Optimum location of one control force. It is easy to prove that the optimum location of one control force based on above two criteria is the top location of a tall building.

(3) Optimum locations of two control forces. This one is complete, detailed analysis can be found from [3]. An example shows that the optimum locations of two control forces are the points of the largest displacement and the second large displacement if the values of two forces are the same. The effect of optimum locations is 2-10 times than that of non-optimum locations.

3. Controlled Structures.

The concept of controlled structures was proposed by Li in 1987. The difference between structural control and controlled structures is that a controlled structure treats the structure and control equipment including active, or passive, or semi-active control or both of them as a large system to conduct optimum design, which is more difficult than that of structural control because the number of non-known parameters of a structure is very large. Several examples of controlled structures were given in book [3].

D. Reliability of Structures

Our contributions are as follows [4]:

1. Analysis for dynamic reliability of aseismic structures.
2. Analysis for static and dynamic reliability of wind resisting structures.
3. Analysis for dynamic reliability of Three Gorge Dam.
4. Time-dependent reliability of engineering structures.

References

[1] Guiqing Li, Calculating Theory and Its Applications of Aseismic Structures, Publishing House of Earthquake, China, 1985

[2] Guiqing Li, Statistic Mathematics, Publishing House of Building Industry, China, 1998

[3] Guiqing Li and Jiayun Xu, Calculating Theory and Its Applications of Structural Control and Controlled Structures, Publishing House of Earthquake, China, 1996

[4] Guiqing Li and Qiusheng Li, Theory and Applications of Time-Dependent Reliability of Engineering Structures, Publishing House of Sciences, China, 2001

Digital Content Analytics and Computational Science

by Fionn Murtagh, Member EUAS

Short Biography

Fionn's initial degrees, BAI and BA, were in Engineering Science and Mathematics, then an MSc in Computer Science, on information retrieval, from Trinity College Dublin, and a PhD (Doctorat de 3ème Cycle) in Mathematical Statistics in Université P&M Curie, Paris 6. The doctorate was with the national geological centre, BRGM, Bureau de Recherches Géologiques et Minières, Orléans. Later he achieved an HDR, Habilitation à Diriger des Recherches, at the Université de Strasbourg, on pattern recognition methods in astronomy.

Fionn's summer positions as a second level student included some months each summer in the national train engineering and production centre in Dublin, including a wide range of production and maintenance; in the Guinness brewery, in the Cadbury chocolate and food factory, in Dublin, and in Brown Boveri & Cie, in Baden, CH, which later merged with Asea to become ABB, Asea Brown Boveri.

Fionn's very first full time position was as Statistician-Programmer in educational research in the Educational Research Centre, in Dublin, working on national level ability and attainment performance evaluation. Following nearly four years as Lecturer in Computer Science in University College Dublin, Fionn was a Visiting Scientist in nuclear reactor safety, data analytics, at the Joint Resarch Centre, Ispra (Varese), Italy. For 12 years Fionn served with the Space Science Department, Astrophysics Division, of the European Space agency, working at the European Southern Observatory in Garching, Munich, on the Hubble Space Telescope project.

Professor of Computer Science posts in the University of Ulster and Queen's University Belfast, followed by Royal Holloway, University of London from 2004, where Fionn was Head of Department in 2005-2007. In 2007-2012, Fionn was Director of ICT and emerging technologies, including engineering and mathematics, computer science, opto-electronics, nanotechnology, and many other domains, and with responibility for sustainable energy research at Science Foundation Ireland.

Fionn is an Honorary Professor in Royal Holloway University of London. Fionn was Head of the School of Computer Science and Informatics in De Montfort University. After that there were joint appointments (0.8 and 0.2) as Professor of Data Science in the University of Derby, and in Goldsmiths University of London. Now Fionn is Professor of Data Science in the University of Huddersfield, and is the Director of the, to be established, Institute of Mathematics and Data Science, that will be very like the model of a Fraunhofer Institute.

Fionn's publications include about 30 books, as author or editor; about 300 journal papers and other refereed publications as book chapters and as conference proceedings. His Google Scholar h-index is 55.

Fionn was Editor-in-Chief, The Computer Journal (British Computer Society, OUP) for more than 10 years and is currently Section Editor for Computational Intelligence, Machine Learning and Data Analytics. He is also on the Editorial Boards of: Journal of Classification (Springer),

Neurocomputing (Elsevier), formerly for Pattern Recognition (Elsevier), formerly also for International Journal of Software and Informatics (Chinese Academy of Sciences), p-Adic Numbers, Ultrametric Analysis and Applications (Russian Academy of Sciences, Springer), Big Data and Cognitive Computing (MDPI), PeerJ Computer Science (PLoS, Public Library of Science), Language and Psychoanalysis, International Review on Computers and Software (IRECOS), Journal of Imaging (MDPI), formerly Journal of Multivariate Analysis (Academic), Artificial Intelligence Review, and other journals. He is book series editor for: Computer Science & Data Analysis (Chapman & Hall/CRC).
Fionn is an elected Member of the Royal Irish Academy, and of Academia Europaea; Fellow of the British Computer Society, of the International Association of Pattern Recognition, of the Institute of Mathematics and Its Applications, and the Royal Society of Arts. He is a member of UKCRC (UK Computing Research Committee), and served on its executive. He was President of the Classification Society (North America), of the British Classification Society (he is now Secretary), has been a Council member of the International Association for Statistical Computing. He is Chair of the Board of the Council for Frontiers of Knowledge, Makerere University, Uganda. Fionn is a Board member of the Classification Society, and is now a Board member of the European Association of Data Science. Fionn is a Senior Member of IEEE, many decades a member of ACM, of the Gesellschaft für Informatik, of the Gesellschaft für Klassifikation, and is a member of the London Mathematical Society, of the Open Data Institute, of the Research Data Alliance, of Engineers Ireland, and many other professional societies. Fionn is a Senior Fellow of the Higher Education Academy, SF HEA, for his teaching. Teaching has been in Ireland, Northern Ireland and England, in France (Observatoire Astronomique, Université de Strasbourg) and in the US (summer course in the University of Washington), and summer courses in Italy, Morocco, Japan, Estonia, and Romania.

Research

Fionn's research is in Digital Content Analytics; Computational Science (including innovative models and paradigms from digital humanities and quantitative social sciences); High Performance Search and Discovery (in massive, high dimensional information spaces, linear and constant computational time algorithms); Narrativization; Multivariate Data Analysis Software; Image and Signal Processing – Multiscale Morphological Modelling.

Fionn's proudest accomplishment: that his doctoral genealogy, from Jean-Paul Benzécri, includes representatives of the Bourbaki movement, and then, going back further, Borel, Lebesgue, Lagrange, Laplace, Euler, the Bernoullis, Leibniz and Huygens.

Fionn has been a partner in many funded research projects, Framework Programme projects at European level, he led COST Action and European Science Foundation projects and UK research council projects on Astrogrid (Big Data in astronomy), civil engineering construction, and projects with national statistics offices (integrating data sources). The company he established, Multi Resolutions Ltd., covers image and signal processing, and also survey analysis. Among the many conferences that Fionn is involved in, organisationally, each year, including sometimes giving keynote presentations, there are these to mention: in 2018 (ECDA 2018, European Conference on Data Analysis), organiser of the session on "Data Science for Mental Health", and chair of the Classification Society's "Distinguished

Dissertation Award", for PhD theses, and chair of the SLDS (Statistical Learning and Data Science) "Jean-Paul Benzécri Prize" award for young researchers.

Outstanding Contributions to Astrostatistics Award 2016, awarded by: IAA Awards, International Astrostatistics Association, with the commendation: "For his long time contributions to astroinformatics and related areas in the computational sciences; advancing scientific knowledge in classification theory and image analysis; for his contributions to the success of the Hubble Space Telescope; for his role on the organizing committee of the IAU Commission B3 on Astroinformatics Astrostatistics; and for his long time efforts in dealing with the statistical analysis of "Big Data"."

Fionn's two most recent books are as follows, and he is engaged with this also: Big Data Clinical Study and Its Implementation with R, AME Publishing Company, China.

Murtagh, F., Data Science Foundations: Geometry and Topology of Complex Hierarchic Systems and Big Data Analytics, Chapman & Hall, CRC Press, 2017.

Starck, J.-L., Murtagh, F. and Fadili, J., Sparse Image and Signal Processing: Wavelets, Curvelets, Morphological Diversity, Cambridge University Press, 2010. 2nd edition, Jan. 2016.

Advanced Materials for Energy Storage & Conversion

by Zongping Shao, Member EUAS

Short Biography

Professor Zongping Shao received his PhD from Dalian Institute of Chemical Physics, Chinese Academy of Sciences in 2000. After that he has been a visiting scholar at the Institut de Researches Sur La Catalyse, CNRS, France and a postdoctoral fellow at California Institute of Technology, USA from March 2002 till June 2005. In July 2005, he joined Nanjing Tech University where he was promoted to a professor. Currently, he is joint-appointed by Nanjing Tech University and Curtin University.

Research Activities and Publications

Professor Shao's research interests include oxygen permeable membranes, solid oxide fuel cells (SOFCs), oxygen reduction, oxygen evolution and hydrogen evolution reactions (ORR, OER and HER), lithium-ion batteries, supercapacitors, polymer-electrolyte membrane fuel cells, solar cells, etc. He has published more than 400 international journal papers with a total citation of >17000 (Google Scholar) and an H-index of 62 (Google Scholar).

Awards

1995 Excellent Undergraduate Student of Hangzhou University
2000 President Prize of Chinese Academy of Sciences
2001-2002 K. C. Wong Education Foundation for Young Chinese Researchers Abroad
2008 Fok Ying-Tong Education Foundation for Young Teachers
2007&2008 The Most Cited Papers from Chinese Researchers, Chinese Ministry of Science & Technology
2008 New Century Distinguished Youths Award, Chinese Ministry of Education
2010 Two Papers as Top Cited Papers for the Period 2006-2010 Published by Chinese Researchers, by Acta Materialia
2010 Distinguished Researchers of China under Age 45 by National Science Foundation of China
2011 Australian Research Council (ARC) Future Fellowship
2011 Changjiang Scholars Program, Chinese Ministry of Education
2013 Distinguished Award for Novel Materials and Their Synthesis by IUPAC& NMS
2014 Thomson Reuters Highly Cited Researcher in Section Engineering
2015 The Top One on the List of Most Cited Chinese Researchers Announced by Elsevier Scopus Data
2015 The Second Prize in Jiangsu Province Science and Technology Award
2016 One of Most Cited Researchers in both Energy Science and Engineering, and Materials Science and Engineering by Elsevier Scopus Data
2016 Special Government Allowances of the State Council

Major Research Areas

1. Mixed conducting membranes for the oxygen permeation

2. Key materials for SOFCs

3. Electrocatalysts for the ORR, OER and HER

4. Lithium-ion batteries and supercapacitors

Typical Researches

$Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ (BSCF), a mixed oxygen-ionic and electronic conductor, was initially developed by Z. P. Shao as a ceramic membrane for oxygen separation from air. In 2004, Z. P. Shao applied BSCF, for the first time, as a cathode material for SOFCs operated below 600 °C when he was the postdoctoral fellow at California Institute of Technology. After that, extensive research has been conducted on intermediate temperature (IT)-SOFCs all over the world encouraging by the exciting results of Z. P. Shao. Actually BSCF has become the hottest cathode material of IT-SOFCs nowadays. This is clearly indicated by the high citations of the paper (*Nature*, 2004, *431*, 170-173; 1742 times until September 2017). Afterward, Prof. Shao's group continues to develop more innovative cathode materials for IT-SOFCs, for example, $SrSc_{0.2}Co_{0.8}O_{3-\delta}$, $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$ and $PrBaCo_2O_{5+\delta}$. The operation temperature of SOFCs was further reduced to the range of 400-600 °C, promoting the development of low-to-intermediate SOFCs.

The improvement of nickel-based anodes for coking/sulfur resistance was also exploited. Prof. Shao found that the coking/sulfur resistance could be significantly improved when a water-storable proton-conducting perovskite oxide was used as the ceramic phase in the nickel cermet-based anode. The as-stored water in the proton-conducting phase can rapidly eliminate carbon/sulfur that was deposited over the nickel surface, leading to the regeneration of the nickel surface in time and the prevention of the carbon/sulfur accumulation. Furthermore, the potential of combining nanocatalysts and water-storable materials in advanced anode catalysts for SOFCs was demostrated by using a facile impregnation and limited reaction protocol. The hierarchical anode composed of nickel nanoparticles, water-storable $BaZr_{0.4}Ce_{0.4}Y_{0.2}O_{3-\delta}$ perovskite and amorphous BaO exhibited high hydrogen electro-oxidation activity, excellent operational stability, superior sulfur tolerance, and good thermal cyclability.

For the room-temperature ORR, Prof. Shao introduced an effective strategy to boost the electrocatalytic activity of palladium (Pd) by stabilizing its unusual oxidation states. $LaFe_{1-x}Pd_xO_3$ ($x = 0.05$ and 0.1) perovskite oxides (containing perovskite-type ionic, $Pd^{3+/4+}$) were created by doping Pd into perovskite oxide lattice. They exhibited higher mass activity, better durability and higher tolerance to methanol than the benchmark Pt/C (platinum supported on carbon) catalyst. Apart from cation doping, the introduction of an A-site cation deficiency presented another approach to enhance the ORR activity of $LaFeO_3$ due to the creation of oxygen vacancies and a small amount of Fe^{4+} species on the perovskite surface.

BSCF, which was formerly known as a high-performance perovskite in oxygen permeation membranes and SOFCs, has been identified as a highly active OER catalyst that even outperforms the gold-standard IrO_2 in terms of intrinsic activity. Based on the design principle for OER electrocatalysts (unit e_g occupancy of B-site cations) and the targeted co-doping strategy, Prof. Shao developed several highly active and stable electrocatalysts for the OER such as $SrNb_{0.1}Co_{0.7}Fe_{0.2}O_{3-\delta}$, $SrSc_xNb_yCo_{1-x-y}O_{3-\delta}$, and

$BaCo_{0.9-x}Fe_xSn_{0.1}O_{3-\delta}$ in the past three years, which even show higher OER activities than BSCF. In a departure from the conventional doping approach utilizing metal elements, non-metal element (phosphorus) doping provides an attractive avenue to optimize the structural stability and OER performance of $SrCoO_{3-\delta}$ perovskite oxide.

Very recently, Prof. Shao found that perovskite oxides can also be developed to efficient HER catalysts through the tuning of their surface electronic structures and properties. To start from BSCF, the most popular perovskite oxides in OER, a highly efficient HER electrocatalyst was obtained through the simple A-site praseodymium (Pr) doping of BSCF. At an optimized Pr-doping concentration, $Pr_{0.5}(Ba_{0.5}Sr_{0.5})_{0.5}Co_{0.8}Fe_{0.2}O_{3-\delta}$ exhibited the highest HER activity in alkaline electrolyte, which favorably compares with that of other non-Pt HER electrocatalysts.

For supercapacitors, Prof. Shao designed and characterized perovskite-type $SrCo_{0.9}Nb_{0.1}O_{3-\delta}$ (SCN) as a novel anion-intercalated electrode material in an aqueous KOH electrolyte, showing high capacitance, excellent rate capability and favorable cycling stability. Furthermore, when coupled with an activated carbon (AC) electrode, the SCN/AC asymmetric supercapacitor (ASC) delivered superb energy density, outperforming most of reported ASCs. This suggests that SCN has potential to be a promising electrode material for next-generation supercapacitors.

Career-Best Research Outputs

[1] **Shao, Z.P.**; Yang, W.S.; Cong, Y.; Dong, H.; Tong, J.H.; Xiong, G.X.; **J. Membr. Sci.**, 172, **2000**, 177-188.
[2] **Shao, Z.P.**; Haile, S.M.; **Nature**, 431, **2004**, 170-173.
[3] **Shao, Z.P.**; Haile, S.M.; Ahn, J.; Ronney, P.; Zhan, Z.L.; Barnett, S.A.; **Nature**, 435, **2005**, 795-798.
[4] **Shao, Z.P.**; Zhang, C.M.; Wang, W.; Su, C.; Zhou, W.; Zhu Z.H.; Park, H.J.; Kwak, C.; **Angew. Chem. Int. Ed.**, 50, **2011**, 1792-1797.
[5] **Shao, Z.P.**; Zhou, W.; Zhu, Z.H.; **Prog. Mater. Sci.**, 57, **2012**, 804-874.
[6] Wang, W.; Su, C.; Wu, Y.Z.; Ran, R.; **Shao, Z.P.**; **Chem. Rev.**, 113, **2013**, 8104-8151.
[7] Yang, B.B.; Ran R.; Zhong, Y.J.; Su, C.; Tadé, M.O.; **Shao, Z.P.**; **Angew. Chem. Int. Ed.**, 54, **2015**, 3722-3725.
[8] Zhu, Y.L.; Zhou, W.; Chen, Z.G.; Chen, Y.B.; Su, C.; Tadé, M.O.; **Shao, Z.P.**; **Angew. Chem. Int. Ed.**, 54, **2015**, 3897-3901.
[9] Zhu, Y.L.; Zhou, W.; Chen, Y.B.; Yu, J.; Liu, M.; **Shao, Z.P.**; **Adv. Mater.,** 27, **2016**, 7150-7155.
[10] Zhu, Y.L.; Zhou, W.; Chen, Y.B.; **Shao, Z.P.**; **Angew. Chem. Int. Ed.**, 55, **2016**, 8988-8993.
[11] Xu, X.; Chen, Y.B.; Zhou, W.; Zhu, Z.H.; Su, C.; Liu, M.; **Shao, Z.P.**; **Adv. Mater.,** 28, **2016**, 6442-6448.
[12] Zhao, B.; Deng, X.; Ran, R.; Liu, M.; **Shao, Z.P.**; **Adv. Energy Mater.,** 6, **2016**, 1500924.
[13] Zhu, L.; Liu, Y.; Su, C.; Zhou, W.; Liu, M.; **Shao, Z.P.**; **Angew. Chem. Int. Ed.,** 55, **2016**, 9576-9579.
[14] Zhu, Y.L.; Zhou, W.; Zhong, Y.J.; Bu, Y.; Chen, X.; Zhong, Q.; Liu, M.; **Shao, Z.P.**; **Adv. Energy Mater.,** 7, **2017**, 1602122.
[15] Liu, Y.; Wang, Z.; Zhong, Y.J.; Tade, M.O.; Zhou, W.; **Shao, Z.P.**; **Adv. Funct. Mater.,** 27, **2017**, 1701229.

New Aspects in Cardiovascular Research & Echocardiography

by Thomas F. Lüscher, Member EUAS

Short Biography

Training and Current Position

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

Clinical Competence and Activity

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

Research

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

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

Research Topics of Professor Thomas F. Lüscher, MD, FESC, FACC; FRCP

Applied Basic Research

The research of the *Center for Molecular Cardioloogy* focuses on the the role of endothelium-derived mediators (i.e. nitric oxide, reactive oxygen species, prostaglandin H2, endothelin-1 and tissue factor) in the regulation of vascular tone, plateletvessel wall interaction, coagulation (tissue factor) as well as vascular structure under physiological conditions and in hypertension, high LDL- and low HDL-cholesterol and atherosclerosis (LOX-1) using cellular and molecular techniques as well as genetically engineered animal models. More recently, aging (p66shc) and longevity genes (Sirtuines, jun-D) have been studied.

Clinical Research

The clinical research aims to translate of basic findings and focusses on vascular dysfunction in patients with hypertension, hyperlipidemia, coronary artery disease and congestive heart failure and employs plethysmography, ultrasound, angiography, IVUS, optical coherence tomography, positron emission tomography and magnetic resonance imaging. In particular, the effects of nutritional and pharmacological interventions and of devices and catheter-based interventions are investigated.

Registries

The natural history is investigated in large registries such as acute coronary syndromes (SPUM –Registry; n =4’700 together with 4 Swiss Centers) and the Tako Tsubo Registry (InterTAK Registry; n = 1’800; together with Christian Templin).

Clinical Multicenter Trials

The clinical research center plans and organizes multicenter trials and aims to translate knowledge into clinical practice. Important trials involved endothelial dysfunction in the coronary circulation and its reversal by pharmacotherapy (ENCORE-1 and ENCORE–2) and stents (SIRTAX, COMFORTABLE). Further,

endothelin antagonists in heart failure (HEAT and EARTH) have been investigated. Recently the effects of the CETP-inhibitor dalcetrapib (Dal-VESSEL) and of exetimibe (PANACEA) on endothelial function and of nutritional products (Pycnogenol, Epicathecin) have been studied. A large multicenter trial on the cardiovascular safety of non-steroidal anti-inflammatory drugs has been completed (PRECISION; NEJM 2067). Currently, a large multicenter study on complete vs. incomplete revascularization in STEMI (Multistars Trial; Co-Primary Investigator) and on the effects of everolimus on infarct size in STEMI (Clever-ACS; Primary Investigator) are starting as is a first-in-man trial with a novel stent (BIOVITESSE; Co-Primary Investigator).

Contributions to Rheology and Polymer Processing

by Avraam I. Isayev, Member EUAS

Short Biography

Dr. Avraam I. Isayev is Distinguished Professor Emeritus of Polymer Engineering at The University of Akron and Editor-in-Chief of Advances in Polymer Technology. He is a co-founding faculty member of the department. He received his Ph.D. in Polymer Science and Engineering, Institute of Petrochemical Synthesis of USSR Academy of Sciences, Moscow; M.Sc. in Applied Mathematics, Institute of Electronic Machine Building, Moscow, USSR; M.Sc.in Chemical Engineering, Azerbaijan Institute of Oil and Chemistry, Baku, USSR. Prior to joining the University in 1983, Isayev conducted research at Cornell University, Technion, USSR Academy of Sciences, and State Research Institute of Nitrogen Industry, USSR. His research interests focus in polymer and composite processing, process modeling, rheo-optics, rheology and constitutive equations of polymers, oil products and disperse systems; the injection, co-injection, transfer, compression and gas-assisted injection molding; processing of self-reinforced or in-situ composites based on blends of flexible and thermotropic liquid crystalline polymers; decrosslinking of thermoset plastics, devulcanization of rubbers and in-situ copolymer formation in immiscible blends with the aid of ultrasonic waves; high temperature and high performance composites and nanocomposites; replacement of the petroleum oils in rubbers by modified biobased oils . Isayev has co-authored 3 editions of 1 monograph on rheology, edited or co-edited 8 books, published 262 papers in the referred journals, 35 chapters in books, 8 papers in encyclopedias, 168 papers in conference proceedings. He holds 30 patents. He advised 48 PhD, 41 MS students and 30 postdocs and visiting scientists. He serves on editorial and advisory boards of many journals. His research was featured in the Boston Globe, Plastics Technology, Rubber and Plastics News, AAAS Science Update, Popular Science, Business Week, Architect Magazine, Tire Technology International, PBS TV and other publications around the world. Isayev is the recipient of the Young Scientist Award (Moscow), the OMNOVA Solutions Signature University Award from the OMNOVA Solutions Foundation, The Melvin Mooney Distinguished Technology Award and The Stafford Whitby Award for Distinguished Teaching and Research both from Rubber Division of the American Chemical Society, the Silver Medal from the Institute of Materials (London), the Vinogradov Prize from the G. V. Vinogradov Society of Rheology (Moscow), the NorTech Award given by Crane Publishers, James L. White Award of the Polymer Processing Society and the Society of Plastics Engineers (SPE) International Award. He is SPE Fellow. Rubber World Magazine included him in 125 People and Innovations That Shaped the Rubber Industry. His biography is listed in major Who's Who publications. He was elected to New York Academy of Sciences in 1994 and European Union Academy of Sciences in 2017.

Ultrasonic Devulcanization of Rubbers (1-13) and Crosslinked Plastics (14-20). Among the numerous problems which mankind face in the 21st century the problem of waste utilization including re-processing and re-using of rubber wastes is enormous. Rubber recycling technology is mainly based on burning used tires to recover their caloric value which is only about two times higher than the caloric value of coal. Also, tires are crushed into fine particles for addition to a virgin rubber as a filler. Unique science-based technology was developed and patented involving ultrasonic extrusion processes and equipment. Extensive studies of ultrasonic devulcanization of tire rubbers and other rubber wastes, allowing recovery of rubber materials, so that they can be

shaped, revulcanized and reused. It was shown that ultrasonic waves at certain levels in the presence of heat and pressure within seconds or less are able to break down the three-dimensional network of crosslinked rubbers. The devulcanized rubbers become soft, reprocessable and curable. The process does not require the use of any chemicals. Significant experimental and theoretical studies were carried out to develop the science-based technology and provided the scientific understanding of the novel devulcanization process. The model and mechanism of devulcanization were proposed by considering ultrasonic wave propagation in a moving viscoelastic medium providing high local energy density leading to overstressed chemical bonds causing break up of various crosslinks leading to devulcanization. Extensive experimental and theoretical work was conducted on used tire rubber and various model rubbers which are constituents of the tire rubber. In addition, devulcanization of tire curing bladder, silicone rubber, EPDM roofing membrane and other rubbers and high resiliency flexible polyether based polyurethane foam were studied. Both sulfur and peroxide cured rubbers were devulcanized. The process allows saving of energy needed in making new rubbers and save environment by creating new materials and products from rubber waste. This allows one to solve the problem of environmental sustainability. The developed process is economically feasible, since the ultrasonically devulcanized rubbers are significantly cheaper than the virgin rubbers. The devulcanized rubbers were revulcanized and their properties were studied. The influence of processing conditions on various rubber properties was also investigated. Gel fraction and crosslink density of the devulcanized materials, as well as mechanical properties after revulcanization, were analyzed as a function of processing parameters including flow rate, clearance of the treatment zone, temperature, pressure, and ultrasonic power. The crosslink density of the various devulcanized rubbers was found to correlate uniquely with their gel fraction and independent of parameters characterizing the ultrasonic energy absorbed. Hence, the degree of devulcanization was characterized by just one parameter, such as the crosslink density or gel fraction of the devulcanized rubber. The most comprehensive parameter characterizing the extent of the treatment was found to be the specific acoustic energy consumed per unit mass of the rubber, which according to estimates, adds only one cent into cost of a pound of rubber. The industrial application of this technology has a significant impact on the further expansion of the recycling technology in automotive, shoe, building and tire industries. The single- and twin-screw extruders were developed suitable for recycling industrially important types of rubber used in shoe soles, gaskets, seals, roofing membranes and tire rubbers.

Recycling of crosslinked plastics such as crosslinked polyethylenes (XPEs) is also a major environmental problem. XPEs are used to manufacture storage tanks by rotational and blow molding, films and sheets, wire and cable insulation, pipes, conduits by extrusion and various products by injection molding. Generally, XPEs crosslinked by vinyl silane, peroxide and radiation providing excellent environmental stress crack resistance, very good low-temperature impact strength and good heat resistance. XPEs are not flowable and shapeable upon heating and shearing, making their recycling very challenging problem. Studies led to discovery of novel environmentally friendly decrosslinking process for XPEs recycling via design and manufacturing of novel ultrasonically aided single- (SSE) and twin-screw (TSE) extruders. Studies on XHDPE and XLDPE showed that the process caused preferential breakage of crosslinks, rather than main chains. Torque and pressure in extruders were found to decrease with increase of ultrasonic energy and specific ultrasonic energy consumption decreased with flow rate, making the process economically viable for industrial uses. Mechanical performance of the decrosslinked XHDPE was found to be close or in some cases even higher than those of virgin XHDPE. The melting temperature and crystallinity of the decrosslinked XLDPE increased with the level of ultrasonic energy. Tensile stress-strain behavior of the decrosslinked XLDPE showed a behavior of typical branched PE with shallow or absent yielding and well-developed necking plateau and strain-hardening behavior depending on the crystallinity. Tensile properties of the decrosslinked XLDPE showed a clear dependence on the level of ultrasonic energy. The Young's modulus, stress at break and strain at break increased with ultrasonic energy leveling off at high energy. The model and simulations of ultrasonic decrosslinking extrusion process was proposed. Simulations indicated quantitative predictions for ultrasonic power consumption and qualitative predictions for gel fraction and crosslink density of the decrosslinked XHDPE on process parameters. These findings

provided possibilities to scale up the process and showed that ultrasonically aided extrusion is viable for industrial recycling of crosslinked plastic waste products and also suitable for reuse of wastes generated on the factory floor during product manufacturing.

Self-reinforced or *In-situ* Composites (21-23). The novel process for manufacturing of self-reinforced (*in-situ*) composites based on thermotropic liquid crystalline polymer (LCP)/thermoplastic and LCP/LCP blends was developed. This discovery has subsequently led to extensive worldwide research in this area. It was shown that at certain processing conditions and LCP concentrations, LCP has the ability to form microfibrils or fibers with diameters ranging from 0.1 to 10 micrometers in the thermoplastic matrices during the processing step. The novel process provides self-reinforced composites that exhibit high modulus and mechanical strength, excellent thermal and chemical resistance along with ease of processing. Through this research over 25 years the science based technology of self-reinforced composites was developed identifying processing conditions and polymer pairs for successful fibrillations of various LCPs in thermoplastic matrices. In addition, a patented technology was also proposed for preparation of laminates of self-reinforced composites. This technology is based on the interplay of melting points of components in blends. Furthermore, self-reinforced LCP/LCP blends were manufactured by injection molding process with performance properties of moldings significantly higher than those of any existing thermoplastics.

Ultrasonically Induced *in-Situ* Copolymerization of Polymer Blends (24-31). High power ultrasonic-assisted extrusion process was developed for *in-situ* copolymer formation and compatibilization of immiscible rubber-rubber, plastic-rubber and plastic-plastic blends in the melt state. The process of *in-situ* copolymerization and compatibilization of the blends occurs at the interface at high pressures and a very short residence time (about 10 s) without use of any chemicals. This occurs by ultrasonically initiated chain scission and subsequent recombination reactions at the interfaces of immiscible polymers in blends leading to formation of *in-situ* copolymers. Ultrasonically treated blends revealed the development of interfacial layers, interfacial roughening and indicated significantly improved interfacial adhesion between components over those without treatment. This led to the formation of a stable blend morphology after annealing in the melt state and provided a significant enhancement of the mechanical performance of the *in-situ* compatibilized blends. The enhancement of reactions of transesterification in polyester-polyester blends was also obtained. These findings were supported by means of various spectroscopic techniques and microscopic observations.

Molding Processes of Plastics (32-55) and Rubbers (56-66). Fundamental scientific studies were performed related to development of basic experimental and theoretical understandings of molding processes especially related viscoelastic effects. Specifically, experimental and theoretical studies on development of the frozen-in molecular orientation and residual stresses in injection moldings of amorphous and semicrystalline polymers were carried out. For amorphous polymers, the growth, relaxation and freezing of the flow-induced normal and shear stresses were included during injection molding cycle along with thermal stresses due to cooling. For semicrystalline polymers, in addition the effect of the flow-induced and quescient crystallization on structure development in injection moldings of semicrystalline polymers were included. Based on these developments, a new theoretical approach to simulate anisotropic shrinkage in moldings of amorphous and semicrystalline polymers was proposed. The predictions were verified against an extensive experimental data. For amorphous polymers, the approach was based on use a compressible nonlinear viscoelastic constitutive equation to calculate the residual flow stress tensor components and to relate them to various components of birefringence through use of the stress-optical rule. Contribution of the thermal stresses to birefringence was calculated based on the photoviscoelastic constitutive equation with measured the stress- and strain-optical behavior of polymers in the glassy state and in the transition region from the glassy to rubbery state. The research was also carried out on injection/compression molding. This development made significant contribution toward manufacturing of CD and DVD substrates. Fundamental studies on

injection molding of light guide plates (LGPs) with surface microstructures were performed. A strong correlation between their luminance of LGPs and degree of filling of microstructures and frozen-in birefringence in LGPs was found. In semicrystalline polymers, in addition to the above effects, the flow-induced and quiescent crystallization were included. This research in single component injection molding was extended toward co-injection molding processes to manufacture multilayer products by simultaneous and sequential co-injection molding. Pioneering contributions to development of the science-based technology for injection molding of rubber compounds were made through modeling, simulation and experimental studies. This extensive research was carried out to verify the proposed approach that includes flow along with vulcanization kinetics. Based on this research it was made possible to specify the suitable processing conditions for rubber injection molding to avoid premature curing during cavity filling and to determine the state of cure distribution in molded products. The methodology was proposed to characterize curing kinetics required for successful injection molding of rubbers including incorporation of nonisothermal cavity filling combined with nonisothermal induction time and nonisothermal cure kinetics. This development is currently utilized in many moldflow software for rubber injection molding.

Rheology and Simulation of Viscoelastic Flow (67-74). The first successful viscoelastic and viscoelastic plastic simulations of the two-dimensional planar contraction and expansion flow at Deborah numbers as high as 1000 corresponding to melt flow in polymer processing were developed. This was the long standing scientific problem. Many attempts were made in literature by various research groups to overcome this problem, but they were unable to get solution above Deborah number of the order of one. The proposed approach based on the streamwise integration of governing nonlinear viscoelastic equation for elastic strain tensor was able to overcome this limitation and compared theoretical predictions with experimental data on build up and relaxation of birefringence in converging and diverging flows at high Deborah numbers. Later, this approach was extended to solve the problem of viscoelastic flow in channels with moving boundary, such as occurs in non-return valves of injection molding machines. Furthermore, pioneering experimental and theoretical studies on dynamic behavior of various non-return valves were performed providing their ranking with respect to their ability to close during injection molding of different thermoplastics. The latter provided basis for choosing suitable non-return valves in injection molding machines for various polymers.

Dispersion of Nanofillers via Ultrasonic Compounding Extrusion (75-93). Novel processes for continuous dispersion of nanofillers in thermoplastics and rubbers for manufacturing of nanocomposites using ultrasonically assisted single- and twin-screw extrusion were proposed. Fundamental studies on mixing of carbon nanotubes, carbon nanofibers and various particulate nanofillers, such as nanoclay, carbon black and silica, in thermoplastics and rubbers were carried out. This process is solvent free and uses no surface modification of the nanofillers. The ultrasonically treated nanocomposites show an increase in the viscosity, storage modulus and reduced damping characteristics, as compared to the untreated ones. This indirectly indicates the presence of better dispersion of nanofillers in polymer matrices under ultrasonic treatment. It was established that high power ultrasound is effective in obtaining relatively homogeneous dispersion via breakage of particle agglomerates and bundle of nanofibers and nanotubes, in comparison with extruded untreated ones. Also, a significant enhancement of intercalation and exfoliation of nanoclays was achieved under action of ultrasound during processing in the melt state. Studies indicated a significant reduction in the rheological and electrical percolation threshold, permeability and increase in thermal and electrical conductivities and mechanical performance of nanocomposites containing conductive nanofillers under action of ultrasound in extruders.

Advanced Environmental Solutions for Rubber Compounding (94-98). Nonrenewable petroleum-based plasticizers are widely used to lower the viscosity of rubber compounds, improve processability and decrease cost. However, some popular petroleum-based plasticizers, such as aromatic oils, are considered to be carcinogenic due to the high polycyclic aromatic hydrocarbon (PAH) content. Therefore, renewable bio-based oil such as soybean oil (SO) is recently emerging

as sustainable replacement for petroleum-based plasticizers in rubbers. This is done by modification of SO through the reaction with dienes including dicyclopentadiene (DCPD) converting the C=C double bonds in the SO into cycloaliphatic groups of higher reactivity. The effect of incorporation of modified SO in styrene-butadiene rubber (SBR), chloroprene rubber (CR) and butyl rubber (IIR) containing carbon black (CB), precipitated silica and their mixture and also different curing systems including sulfur, metal oxide and phenolic resin is investigated. Rheological, thermal, dynamic, mechanical and aging properties of rubber compounds containing modified SO are compared with those of virgin SO and a petroleum-based naphthenic oil (NO). Results showed that SO and modified SO can react with various additives such as curatives and silane coupling agent during the curing process and change various properties. Rubbers containing modified SO showed improved elongation at break and tensile strength, cure rate and aging resistance than those with NO and SO. Both SO and modified SO provided rubbers with better thermal stability and lower glass transition temperature than NO. Rubbers containing modified SO also showed dynamic properties suitable for manufacturing tires with better wet traction and lower rolling resistance, and also better abrasion resistance simultaneously compared with those with NO. It is shown that modified SO is a good environmentally friendly replacement for petroleum-based rubber plasticizers in rubber compounds along with improved performance of rubber products and better environmental safety in rubber factories.

References

1. A. I. Isayev, "Continuous Ultrasonic Devulcanization of Vulcanized Elastomers", US Patent 5,258,413, Nov. 2, 1993.
2. A. I. Isayev, J. Chen, "Continuous Ultrasonic Devulcanization of Vulcanized Elastomers", US Patent 5,284, 625, Feb. 8, 1994
3. A. I. Isayev, J. Chen and A. Tukachinsky, "Novel Ultrasonic Technology for Devulcanization of Waste Rubbers", Rubber Chemistry and Technology, 68, 267-280, 1995
4. A. I. Isayev, S. P. Yushanov and J. Chen, "Ultrasonic Devulcanization of Rubber Vulcanizates. Part 1: Process Model", J. Appl. Polym. Sci., 59, 803-813, 1996
5. A. I. Isayev, S. P. Yushanov and J. Chen, "Ultrasonic Devulcanization of Rubber Vulcanizates. Part 2: Simulation and Experiment", J. Appl. Polymer Sci., 59, 815-824, 1996
6. S. P. Yushanov, A. I. Isayev and S. H. Kim, "Ultrasonic Devulcanization of SBR Rubber: Experimentation and Modeling Based on Cavitation and Percolation Theories", Rubber Chemistry and Technology, 71, 168-190, 1998
7. A. I. Isayev, "Rubber Recycling", in Book Rubber Technologist's Handbook, Eds. J. R. White and S. K. De, RAPRA Technology Ltd., UK, Chapter 15, pp. 511-547, 2001
8. S. Ghose and A. I. Isayev, "Continuous Process for Recycling of Polyurethane Foam", J. Cellular Plastics, 40, 3, 167-189, 2004
9. A. I. Isayev and S. Ghose, "Ultrasonic Devulcanization of Used Tires and Waste Rubbers", in book Rubber Recycling, S. K. De, A. I. Isayev and K. Khait, eds., CRC Press, Boca Raton, Chapter 9, pp. 311-384, 2005
10. X. Sun, A. I. Isayev, "Continuous Ultrasonic Devulcanization: Comparison of Carbon-Black- Filled Synthetic Isoprene and Natural Rubbers", Rubber Chemistry and Technology, 81, #1, 38-65, 2008.
11. A. I. Isayev, T. Liang and T. M. Lewis, "Effect of Particle Size on Ultrasonic Devulcanization of Tire Rubber in Twin Screw Extruder," Rubber Chemistry and Technology, 87(1), 86-102 (2014); doi:10.5254/RCT.13.87926.
12. Ivan Mangili, Marina Lasagni, Keyuan Huang and Avraam I. Isayev, "Modeling and optimization of ultrasonic devulcanization using the response surface methodology based on central composite face-centered design," Chemometrics and Intelligent Laboratory Systems, 144, 1-10 (2015); doi: 10.1016/j.chemolab.2015.03.003.
13. Ivan Mangili, Manuela Anzano, Elena Collina, Marina Lasagni, Valeria Tatangelo, Andrea Franzetti, Paola Caracino, Avraam I. Isayev, "Study of Green Devulcanization Technologies Part II: Influence on Properties of Natural Rubber Compounds Containing Devulcanized Ground Tire Rubber from Several Methods," Polymer Degradation and Stability, 121, 369-377 (2015; http://dx.doi.org/10.1016/j.polymdegradstab.2015.10.004.
14. A. I. Isayev and Keyuan Huang, "Decrosslinking of Crosslinked High-Density Polyethylene via Ultrasonically Aided Single Screw Extrusion," Polymer Engineering and Science, 54 (12), 2715–2730 (2014); DOI 10.1002/pen.23827.
15. Keyuan Huang, Avraam I. Isayev and Jing Zhong, "Ultrasonic Decrosslinking of Crosslinked High-Density Polyethylene: Effect of Screw Design," Journal of Applied Polymer Science, 131(17), 8506-8521 (2014); DOI: 10.1002/app.40680. ISSN: 0021-8995.
16. Keyuan Huang and Avraam I. Isayev, "Ultrasonic Decrosslinking of Crosslinked High-Density Polyethylene: Effect of Degree of Crosslinking," RSC Advances, 4, 38877-38892 (2014), DOI: 10.1039/c4ra04860a.
17. Keyuan Huang and Avraam I. Isayev, "Comparison between Decrosslinking of Crosslinked High and Low Density Polyethylenes via Ultrasonically Aided Extrusion," Polymer, 70, 290-306 (2015); DOI:10.1016/j.polymer.2015.05.047.
18. Keyuan Huang and Avraam I. Isayev, "Ultrasonic decrosslinking of peroxide crosslinked HDPE in twin screw extrusion: Part I. Process model and simulation," Polymer Engineering and Science, 57 (10), 1035-1046 (2017); DOI 10.1002/pen.24487.
19. Keyuan Huang and Avraam I. Isayev, "Ultrasonic decrosslinking of peroxide crosslinked HDPE in twin screw extrusion: Part II. Experiment and simulation," Polymer Engineering and Science, 57 (10), 1047-1061 (2017); DOI: 10.1002/pen.24470.
20. Avraam Isayev, US Patent 9,714,333; Japanese Patent 5,878,974; European Patent 2,697,032; US Patent Appl. 20170190865.
21. A. I. Isayev, "Self-Reinforced Composites Involving LCP: Overview of Development and Applications", in Book Liquid Crystalline Polymer Systems: Technological Advances, Edited by A. I. Isayev, T. Kyu and D. Cheng, ACS Symposium Series, Washington D. C., No. 632, 1-20 (1996).
22. C. H. Song and A. I. Isayev, "Nanocomposites of Liquid Crystalline Polymerss Dispersed in Polyester Matrices" in book Handbook of Polymer Nanocomposites, Eds. R.K. Gupta, E.B. Kennel and K.J. Kim, CRC Press, Boca Raton, Chapter 11, pp. 253-308, 2010.
23. A. I. Isayev, "Liquid Crystalline Composites", Wiley Encyclopedia of Composites, Edited by L. Nicolais and A. Borzacchiello, 2nd Ed.,Wiley, New York, v. 2, pp. 1468-1496 (2012).

24. Avraam Isayev and Chang Kook Hong, US patent 6,528,554.
25. A. I. Isayev and C. K. Hong, "Novel Ultrasonic Process for *In-situ* Copolymer Formation and Compatibilization of Immiscible Polymers", Polym. Eng. Sci., 43, 91-101, 2003.
26. J. S. Oh, A. I. Isayev and M. A. Rogunova, "Continuous Ultrasonic Process for In-situ Compatibilization of Polypropylene/Natural Rubber Blends", Polymer, 44, 2337-2349, 2003.
27. W. Feng and A. I. Isayev, "In-situ Ultrasonic Compatibilization of PP/EPDM Blends during Ultrasound Aided Extrusion", Polymer, 45, 1207-1216, 2004.
28. A. I. Isayev, S. H. Kim and W. Feng, "Continuous Ultrasonic Treatment of Uncured and Sulfur-Cured SBR: Effect of Styrene Content", Rubber Chem. Technol., 78, no. 4, 606-619 (2005);Rubber Chem. Technol., 78, no. 4, 606-619 (2005).
29. Heng Lin and A. I. Isayev, "Ultrasonic Treatment of Polypropylene, Polyamide 6 and Their Blends during Extrusion", J. Appl. Polym. Sci., 102, 3, 2643-2653 (2006).
30. K. Gunes, A. I. Isayev, X. Li, C. Wesdemiotis, "Fast In-situ Copolymerization of PET/PEN Blends by Ultrasonically Aided Extrusion", Polymer 51, 1071-1081 (2010).
31. K. Gunes and A. I. Isayev, "In-situ Compatibilization of PEN/LCP Blends by Ultrasonic Extrusion", Journal of Applied Polymer Science", 122, 354-365 (2011).
32. A. I. Isayev, Editor "Injection and Compression Molding Fundamentals", Marcel Dekker, Inc., New York, 1987, 703 pp.
33. A. I. Isayev, Editor "Modeling of Polymer Processing - Recent Developments", Hanser Publishers, Munich, 1991, 312 pp.
34. M. R. Kamal, A. I. Isayev and S.-J. Liu "Injection Molding: Technology and Fundamentals", Hanser, Munich, 2009, 926 pp.
35. A. I. Isayev and C. A. Hieber, "Toward a Viscoelastic Modeling of the Injection Molding of Polymers", Rheol. Acta, v. 19, 168-182, 1980.
36. A. I. Isayev, "Orientation, Residual Stresses and Volumetric Effects in Injection Molding", in Book Injection and Compression Molding Fundamentals, Edited by A. I. Isayev, Marcel Dekker, Inc., New York, 227-328 (1987).
37. A. I. Isayev, "Thermal Stresses" in Encyclopedia of Polymer Science and Engineering, John Wiley & Sons, New York, v. 16, pp. 747-767, 1989.
38. N. Famili and A. I. Isayev, "Viscoelastic Modeling of Injection Molding", in book "Modeling of Polymer Processing - Recent Developments", Edited by A. I. Isayev, Hanser Publishers, 247-276 (1991).
39. G. D. Shyu, A. I. Isayev and C. T. Li, "Photoviscoelastic Behavior of Amorphous Polymers during Transition from the Glassy to Rubbery State", J. Polym. Sci., Phys. Ed., 39, 2252-2262, 2001.
40. G. D. Shyu, A. I. Isayev and C. T. Li, "Residual Thermal Birefringence in Freely Quenched Plates of Amorphous Polymers: Simulation and Experiment", J. Polym. Sci., Phys. Ed., 41, 1850-1867, 2003.
41. K. H. Kim, A. I. Isayev and K. H. Kwon, "Flow-induced Crystallization in Injection Molding of Polymers: Thermodynamic Approach", J. Appl. Polym. Sci., 95, 3, 502-523, 2005.
42. A. I. Isayev, G. D. Shyu and C.T. Li, "Residual Stresses and Birefringence in Injection Molding of Amorphous Polymers", J. Polym. Sci., Polym. Phys., 44, 3, 622-639, 2006.
43. K. Kwon, A. I. Isayev and K. H. Kim, "Toward a Viscoelastic Modelling of Anisotropic Shrinkage in Injection Molding of Amorphous Polymers", J. Appl. Polym. Sci., 98, 5, 2300-2313, 2005.
44. K. Kwon, A. I. Isayev, K. H. Kim and C. van Sweden, "Theoretical and Experimental Studies of Anisotropic Shrinkage in Injection Molding of Semicrystalline Polymers", Polym. Eng. Sci., 46, 6, 712-728, 2006.
45. K. Kwon, A. I. Isayev and K. H. Kim, "Theoretical and Experimental Studies of Anisotropic Shrinkage in Injection Moldings of Slow Crystallizing Polymers", J. Appl. Polym. Sci., 102, 4, 3526-3544, 2006.
46. T. H. Lin, A. I. Isayev and M. Mehranpour, "Luminance of Injection Molded V-Groove Light Guide Plates", Polymer Engineering and Science, 48, 8, 1615-1623 (2008).
47. T. H. Lin and A. I. Isayev, "Photoviscoelastic Behavior and Residual Thermal Birefringence in Optical Grade Polycarbonates", Rheologica Acta, 47, 977-988 (2008).
48. A. I. Isayev and K. Kwon, "Volumetric and Anisotropic Shrinkage in Injection Moldings of Thermoplastics", in book Injection Molding: Technology and Fundamentals, Eds. M. R. Kamal, A. I. Isayev and S.-J. Liu, Hanser, Munich, Chapter 19, pp. 779-808, 2009.
49. A. I. Isayev and N. H. Kim, "Co-injection Molding of Polymers", in book Injection Molding, Technology and Fundamentals" Eds. M. R. Kamal, A. I. Isayev and S.-J. Liu, Hanser, Munich, Chapter 21, pp.851-915, 2009.
50. Antonio J. Carrillo and A. I. Isayev, ""Birefringence in Gas-Assisted Tubular Injection Moldings: Simulation and Experiment", Polymer Engineering and Science 49, 12, 2350-2373 (2009).
51. A. I. Isayev and T. H. Lin, "Frozen-in Birefringence and Anisotropic Shrinkage in Optical Moldings: I. Theory and Simulation Scheme", Polymer, 51, 1, 316-327 (2010).
52. A. I. Isayev, T. H. Lin and K. Kwon, "Frozen-in Birefringence and Anisotropic Shrinkage in Optical Moldings: II. Comparison of Simulations with Experiments on Light Guide Plates," Polymer, 51, No. 23, 5623-5639 (2010).
53. Antonio J. Carrillo and A. I. Isayev, "Thermal Stresses and Birefringence in Quenched Tubes and Rods: Simulation and Experiment", Polymer Engineering and Science, 51, #1, 179-200 (2011).
54. Nam Hyung Kim and Avraam I. Isayev, "Birefringence in Injection-Compression Molding of Amorphous Polymers: Simulation and Experiment," Polymer Engineering and Science, 53(8), 1786-1808 (2013).
55. Nam Hyung Kim and Avraam I. Isayev, "Thermal Birefringence in Freely Quenched Multilayered Slabs of Amorphous Polymers: Experiment and Simulation", Polymer Engineering and Science, 54 (9), 2097-2111 (2014); DOI: 10.1002/pen.23748.
56. A. I. Isayev, and J. S. Deng, "Nonisothermal Vulcanization of Rubber Compounds", Rubber Chem. Technol., 61, 340-361, 1988.
57. A. I. Isayev, M. Sobhanie and J. S. Deng, "Two-Dimensional Simulation of Injection Molding of Rubber Compounds", Rubber Chem. Technol., 61, 906-937, 1988.
58. M. Sobhanie and A. I. Isayev, "Viscoelastic Simulation of Flow of Rubber Compounds", Rubber Chem. Technol., 62, 5, 939-956, 1989.
59. M. Sobhanie, J. S. Deng and A. I. Isayev, "Simulation and Experimental Studies of Injection Molding of Rubber Compounds", J. Appl. Polym. Sci., Applied Polymer Symposium, 44, 115-165, 1989.
60. J. S. Deng and A. I. Isayev, "Injection Molding of Rubber Compounds- Experimentation and Simulation", Rubber Chem. Technol., 64, 2, 296-324, 1991.
61. M. Sobhanie and A. I. Isayev, "Simulation of Injection Molding of Rubber Compounds", in Book "Modeling of Polymer Processing - Recent Developments", Edited by A. I. Isayev, Hanser Publishers, 205-246 (1991).
62. A. I. Isayev, R. J. Scavuzzo and Y. Kuroyama, "Injection Molding of Rubber Compounds: Cavity Filling, Packing and Flash Formaton", J. Appl. Polym. Sci., Applied Polymer Symposium, 53, 233-252, 1994;
63. M. Wan and A. I. Isayev, "Injection Molding of Rubber Compound with Rheology Affected by Vulcanization, Part 2: Modeling and

Experiment", Rubber Chemistry and Technology, 69, 294-312, 1996. 64. A. I. Isayev and M. Wan, "Injection Molding of Natural Rubber Compound: Simulation and Experimental Studies", Rubber Chemistry and Technology, 71, 1059-1072, 1998.
65. C. T. Li and A. I. Isayev, "Interface Evolution and Penetration Behavior During Two-component Transfer Molding. Part I: Modeling and Formulation", Polym. Eng. Sci., 44 ,4, 687-696, 2004.
66. C. T. Li, A. I. Isayev and R. L. Warley, "Interface Evolution and Penetration Behavior During Two-component Transfer Molding. Part II: Simulation and Experiment", Polym. Eng. Sci., 44 ,4, 697-713, 2004.
67. A. I. Isayev and R. K. Upadhyay, "Two-Dimensional Viscoelastic Flows, Experimentation and Modelling", J. Non-Newt. Fluid Mech., v. 19, 135-160, 1985.
68. R. K. Upadhyay and A. I. Isayev, "Simulation of Two-Dimensional Planar Flow of Viscoelastic Fluid", Rheol. Acta, v. 25, 80-94, 1986.
69. A. I. Isayev and R. K. Upadhyay, "Flow of Polymeric Melts in Juncture Regions of Injection Molding", in book Injection and Compression Molding Fundamentals, Edited by A. I. Isayev, Marcel Dekker, Inc., New York, 137-225 (1987).
70. Y. H. Huang and A. I. Isayev, "An Experimental Study of Planar Entry Flow of Rubber Compound", Rheol. Acta, 32, 270-276, 1993.
71. A. I. Isayev and Y. H. Huang, "Two-Dimensional Planar Contraction and Expansion Flow of a Viscoelastic Plastic Medium", Rheol. Acta, 32, 181-191, 1993.
72. A. I. Isayev, C. Zook, Y. Zhang, R. J. Scavuzzo, M. Teeple and S. Knoop, "Dynamic Behavior of Various Non-return Valves in Injection Molding Machine, SPE Technical Papers", 41, 595-599 (1995).
73. A. I. Isayev, Y. Zhang and C Zook, "Flow of Polymeric Melts in Channels with Moving Boundaries" in Book Advances in the Flow and Rheology of Non-Newtonian Fluids, Edited by D. A. Siginer, D. DeKee and R. P. Chhabra, Elsevier Science, Amsterdam, 1011-1067 (1999).
74. Chris Zook and A. I. Isayev, "Simulation and Experimental Studies of a Non-return Valve Performance during Injection Molding", J. Injection Molding Technology, 4, 65-77, 2000.
75. A. I. Isayev and S. Lapshin, US Patent Application 20060148959 published on July 6, 2006 (filed as provisional application on May 2005 and filed January 2006).
76, A. I. Isayev, S. Lapshin and S. K. Swain, "Process for Preparing Polymer Nanocomposites and Nanocomposites Prepared Therefrom", US Patent Application,# 20100152325, Application Serial No. 11/823,023 was filed 6/26/2007.
77. A. I. Isayev ,"Ultrasound Assisted Continuous Process for Dispersion of Nanofibers and Nanotubes in Polymers," US # 20090275689 Filed June 5, 2007, published November 5, 2009;
78. S. Lapshin and A. I. Isayev, "Continuous Process for Melt Intercalation of PP-Clay Nanocomposites with Aid of Power Ultrasound", J. Vinyl Additive Technol., 12, 78-82 (2006).
79. S. Lapshin, A. I. Isayev, "Ultrasound Aided Extrusion Process for Preparation of Polypropylene-Clay Nanocomposites", J. Vinyl Additive Technol., 13, 40-45 (2007).
80. H. Tan and A. I. Isayev, "Comparative Study of Silica-, Nanoclay- and Carbon Black- Filled EPDM Rubbers Treated by Ultrasound", Rubber Chemistry and Technology, 81, #1, 157-174 (2008);
81. S. Lapshin, S. K. Swain and A. I. Isayev, "Ultrasound Aided Extrusion Process for Preparation of Polyolefin-Clay Nanocomposites", Polymer Engineering and Science, 48, 8, 1584-1591 (2008).
82. A. I. Isayev, C. Jung, K. Gunes and R. Kumar, "Ultrasound Assisted Single Screw Extrusion Process for Dispersion of Carbon Nanofibers in Polymers", Intern. Polym. Process., 23, 4, 395-405 (2008).
83. A. I. Isayev, R. Kumar and T. M. Lewis, "Ultrasound Assisted Twin Screw Extrusion of Polymer Nanocomposites Containing Carbon Nanotubes", Polymer, 50, 250-260 (2009).
84. S. K. Swain and A. I. Isayev, "PA6/Clay Nanocomposites by Continuous Sonication Process", Journal of Applied Polymer Science, 114, 4, 2378-2387 (2009).
85. R. Kumar and A. I. Isayev, "Thermotropic LCP/CNF Nanocomposites Prepared with Aid of Ultrasonic Waves", Polymer, 51, 3503-3511 (2010).
86. J. Choi and A. I. Isayev, "Ultrasonic Aided Extrusion of Carbon Black Filled SBR Compounds", Rubber Chemistry and Technology, 84, #1, 55-73. (2011).
87. S. Niknezhad and A. I. Isayev, "Online Ultrasonic Film Casting of LLDPE and LLDPE/Clay Nanocomposites," Journal of Applied Polymer Science, (DOI: 10.1002/app.38725), 129 (1), 263-275 (2013).
88. Jing Zhong, Avraam I. Isayev, Keyuan Huang, "Influence of ultrasonic treatment in PP/CNT composites using masterbatch dilution method," Polymer, 55(7), 1745-1755 (2014). DOI: 10.1016/j.polymer.2014.02.014. ISSN: 0032-3861.
89. Xiang Gao, Avraam I. Isayev and Chao Yi, "Ultrasonic treatment of polycarbonate/carbon nanotubes composites," Polymer, 84, 209-222 (2016).
90. Jing Zhong, Avraam I. Isayev, Xiaoping Zhang, "Ultrasonic twin screw compounding of polypropylene with carbon nanotubes, graphene nanoplates and carbon black," European Polymer Journal, 80, 16-39 (2016).
91. Jing Zhong and Avraam I. Isayev, "Ultrasonically assisted compounding of CNT with polypropylenes of different molecular weights," Polymer, 107, 130-146 (2016); http://dx.doi.org/10.1016/j.polymer.2016.11.006
92. Xiang Gao, Avraam I. Isayev, Xiaoping Zhang, Jing Zhong, "Influence of processing parameters during ultrasonic extrusion on the properties of polycarbonate/carbon nanotubes composites," Composite Science and Technology, 144, 125-138 (2017); http://dx.doi.org/10.1016/j.compscitech.2017.03.019
93. Jing Zhong and Avraam I. Isayev, "Ultrasonic treatment of PP/CNT composites during twin-screw extrusion: effect of screw configuration," Polymer Composites, 38 (12), 2695-2706 (2017); DOI 10.1002/pc.23867.
94. Jiaxi Li, Avraam I. Isayev, Xiaofeng Ren and Mark D. Soucek, "Modified Soybean Oil-Extended SBR Compounds and Vulcanizates Filled with Carbon Black," Polymer, 60, 144-156 (2015); http://dx.doi.org/10.1016/j.polymer.2015.01.028.
95. Jiaxi Li, Avraam I. Isayev, Xiaofeng Ren and Mark D. Soucek, "Effect of norbornyl modified soybean oil on CB-filled chloroprene rubber," Journal of Applied Polymer Science, 133 (33), 43809 (1 of 10) (2016); DOI: 10.1002/APP.43809.
96. Jiaxi Li, Avraam I. Isayev, Xiaofeng Ren and Mark D. Soucek "Toward Replacement of Petroleum Oils by Modified Soybean Oils in Elastomers," Rubber Chemistry and Technology, 89 (4), 608-630 (2016). http://dx.doi.org/10.5254/rct.16.84830
97, Jiaxi Li, Avraam I. Isayev, Xiaofeng Ren, Mark D. Soucek, "Norbornylized Soybean Oil as Sustainable New Plasticizer for Rubbers with Hybrid Fillers," Polymer International, 66, 820-829 (2017); DOI 10.1002/PI.5321
98. Jiaxi Li, Avraam I. Isayev, Qianhe Wang, Mark D. Soucek, "Sustainable Plasticizer for Butyl Rubber Cured by Phenolic Resin," Journal of Applied Polymer Science, 2017; DOI: 10.1002/APP45500.

Biomedical Materials and Clinical Biochemistry

by Pankaj Vadgama, Member EUAS

Short Biography

CURRENT APPOINTMENTS

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

ACADEMIC QUALIFICATIONS

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

ACADEMIC APPOINTMENTS

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

Editorial Board Positions

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

Chemosensors and biosensors based on polyelectrolyte microcapsules containing fluorescent dyes and enzymes

Kazakova, LI; Shabarchina, LI; Anastasova, S; Pavlov, AM; Vadgama,; Skirtach, AG ; Sukhorukov, GB

ANALYTICAL AND BIOANALYTICAL CHEMISTRY 405 Issue: 5 Pages: 1559-1568 2013

The concept of enzyme-assisted substrate sensing based on use of fluorescent markers to detect the products of enzymatic reaction has been investigated by fabrication of

micron-scale polyelectrolyte capsules containing enzymes and dyes in one entity. Microcapsules approximately 5 mu m in size entrap glucose oxidase or lactate oxidase, with peroxidase, together with the corresponding markers Tris(4,7-diphenyl-1,10-phenanthroline)ruthenium(II) dichloride (Ru(dpp)) complex and dihydrorhodamine 123 (DHR123), which are sensitive to oxygen and hydrogen peroxide, respectively. These capsules are produced by co-precipitation of calcium carbonate particles with the enzyme followed by layer-by-layer assembly of polyelectrolytes over the surface of the particles and incorporation of the dye in the capsule interior or in the multilayer shell. After dissolution of the calcium carbonate the enzymes and dyes remain in the multilayer capsules. In this study we produced enzyme-containing microcapsules sensitive to glucose and lactate. Calibration curves based on fluorescence intensity of Ru(dpp) and DHR123 were linearly dependent on substrate concentration, enabling reliable sensing in the millimolar range. The main advantages of using these capsules with optical recording is the possibility of building single capsule-based sensors. The response from individual capsules was observed by confocal microscopy as increasing fluorescence intensity of the capsule on addition of lactate at millimolar concentrations. Because internalization of the micron-sized multi-component capsules was feasible, they could be further optimized for in-situ intracellular sensing and metabolite monitoring on the basis of fluorescence reporting.

Electropolymerised Phenolic Films as Internal Barriers for Oxidase Enzyme Biosensors

Spehar-Deleze, AM; Anastasova, S; Vadgama, P ELECTROANALYSIS 26 Issue: 6 Pages: 1335-1344 Special Issue: SI 2014

The properties of electropolymerised phenolic films at amperometric needle electrodes were investigated and their applicability as selective, internal barriers for potential in vivo oxidase enzyme based biosensors evaluated. Polyphenol, poly(phenol red) and dual layer poly(phenol red)/poly(4-aminophenol) films were formed by electropolymerisation and compared with a solvent deposited sulfonated polyether ether sulfone-polyether sulfone (SPEES-PES) membrane. Phenol red had two distinct cyclic voltammetry peaks on platinum: an oxidative peak at +0.70 V and a reduction peak at -0.2 V vs. Ag/AgCl, respectively. Also, the film enhanced the oxidation of hydrogen peroxide by a factor of 3-4, making it an attractive barrier for oxidase based biosensors. Lactate sensors made with polyphenolic electropolymers and solvent deposited SPEES/PES were compared for selectivity and lactate response; the latter showed better selectivity against acetaminophen but less selectivity against ascorbic acid. When sensors were sterilised by standard gamma irradiation for in vivo application, the polyphenolic films degraded and lost selectivity, whilst SPEES/PES survived unchanged. Salivary lactate was monitored during exercise with electropolymerised film sensors and demonstrated mean lactate increases of 0.3-0.6 mM.

Study of albumin and fibrinogen membranes formed by interfacial crosslinking using microfluidic flow

Chang, H; Khan, R; Rong, ZM; Sapelkin, A ; Vadgama, P

BIOFABRICATION Volume: 2 Issue: 3 Article Number: 035002 2010

Microfluidics enables scale reduction in sample volume with obvious benefits for reagent conservation. In contrast to conventional macro-scale flow, microfluidics also offers unprecedented control over flow dynamics. In particular, laminar flow is readily achieved, allowing for new analytical and synthetic strategies. Here, two parallel flows of buffer and xylene were used to create a stable liquid-liquid interface within linear micro-

channels. These, respectively, carried protein (albumin or fibrinogen) and an acyl chloride to effect protein crosslinking. This created robust, micro-membranes at the interface that bisected the fluid channel. Membrane formation was self-limiting, with fibrinogen membranes showing greater solute permeability than albumin, based on dye transport (Ponceau S, Meldola Blue). The crosslinker isophthaloyl dichloride led to thinner, less permeable membranes than terephthaloyl chloride. Larger surface area membranes formed at a static liquid-liquid interface served as a more physically accessible model and allowed precise electrochemical determination of acetaminophen, catechol and peroxide diffusion coefficients, which confirmed the greater fibrinogen permeability. Scanning electron microscopy (SEM) of the membranes also indicated a higher population of discrete nanopores at the fibrinogen surface. A crosslinking pH had a strong effect on overall permeability. Adhesion of B50 neuronal cells was demonstrated, and it is proposed that the membranes could facilitate cell growth through bidirectional nutrient supply in a micrbioreactor format.

3D Printed Microfluidic Device with Integrated Biosensors for Online Analysis of Subcutaneous Human Microdialysate

Gowers, SAN; Curto, VF; Seneci, CA ; Wang, C; Anastasova, S; ; Vadgama, P; Yang, GZ; Boutelle, MG

ANALYTICAL CHEMISTRY Volume: 87 Issue: 15 Pages: 7763-7770 2015

This work presents the design, fabrication, and characterization of a robust 3D printed microfluidic analysis system that integrates with FDA-approved clinical microdialysis probes for continuous monitoring of human tissue metabolite levels. The microfluidic device incorporates removable needle type integrated biosensors for glucose and lactate, which are optimized for high tissue concentrations, housed in novel 3D printed electrode holders. A soft compressible 3D printed elastomer at the base of the holder ensures a good seal with the microfluidic chip. Optimization of the channel size significantly improves the response time of the sensor. As a proof-of-concept study, our microfluidic device was coupled to lab-built wireless potentiostats and used to monitor real-time subcutaneous glucose and lactate levels in cyclists undergoing a training regime.

Modulation of cell growth on exposure to silkworm and spider silk fibers

Hakimi, O; Gheysens, T; Vollrath, F; Grahn, MF; Knight, DP; Vadgama, P

JOURNAL OF BIOMEDICAL MATERIALS RESEARCH PART A Volume: 92A Issue: 4 Pages: 1366-1372

2010

Recent years have seen an increased interest in the use of natural and modified silks for tissue engineering. Despite longstanding concerns regarding the biocompatibility of silk sutures, only a few studies have been carried out to investigate the biocompatibility of natural silk fibers. Here, we report an in vitro assessment of the effect of nonmodified, degummed silks on cells. We describe the effects of degummed silk fibers as well as extracted sericin on cell metabolism and proliferation. Endothelial cells directly exposed to native degummed Bombyx mori and Antheraea pernyi silks showed lower rates of proliferation and metabolism than nonexposed cells. A similar but milder effect was observed for cells in direct contact with Nephila edulis egg sack fibers. Sericin and silk-conditioned medium had no negative effect on cell proliferation except in medium supplemented with 5% bovine serum prior to conditioning with A. pernyi silk. The toxicity of A. pernyi was negligible after thorough enzymatic treatment of the fibers with trypsin. It

is, therefore, proposed that A. pernyi silk contain one or more cytotoxic components, which need to be removed prior to medical use.

Electrochemical determination of microRNAs based on isothermal strand-displacement polymerase reaction coupled with multienzyme functionalized magnetic micro-carriers

Ma, W; Situ, B; Lv, WF; Li, B; Yin, XM; Vadgama, P; Zheng, L ; Wang, W
BIOSENSORS & BIOELECTRONICS Volume: 80 Pages: 344-351 2016

MicroRNAs (miRNAs) show great potential for disease diagnostics due to their specific molecular profiles. Detection of miRNAs remains challenging and often requires sophisticated platforms. Here we report a multienzyme-functionalized magnetic microcarriers-assisted isothermal strand-displacement polymerase reaction (ISDPR) for quantitative detection of miRNAs. Magnetic micro-carriers (MMCs) were functionalized with molecular beacons to enable miRNAs recognition and magnetic separation. The target miRNAs triggered a phi29-mediated ISDPR, which can produce biotin-modified sequences on the MMCs. Streptavidin-alkaline phosphatase was then conjugated to the MMC surface through biotin-streptavidin interactions. In the presence of 2-phospho-L-ascorbic acid, miRNAs were quantitatively determined on a screen-printed carbon electrode from the anodic current of the enzymatic product. We show that this method enables detection of miRNAs as low as 9 fM and allows the discrimination of one base mismatched sequence. The proposed method was also successfully applied to analyze miRNAs in clinical tumor samples. This paper reports a new strategy for miRNAs analysis with high sensitivity, simplicity, and low cost. It would be particularly useful for rapid point-of-care testing of miRNAs in clinical laboratory.

An electrochemical study of microporous track-etched membrane permeability and the effect of surface protein layers

Adatia, K; Raja, M; Vadgama, P
COLLOIDS AND SURFACES B-BIOINTERFACES Volume: 158 Pages: 84-92 2017

Microporous track-etched membranes serve as important permeable growth surfaces for cell culture where diffusive solute transport is needed across two growth compartments. This study has established effective solute diffusion coefficients for four probe micro-solutes: hydrogen peroxide, pyrocatechol, acetaminophen and ascorbic acid across three track-etched membranes formulated, respectively, from polycarbonate and polyethylene terephthalate. Chronoamperometry and cyclic voltammetry were used for the diffusion measurements. These showed substantially reduced intra-pore diffusion in relation to available pore area. Diffusion coefficients ranging from 1.43 x 10(-10) to 3.17 x 10(-7) cm(2) s(-1) were demonstrated. This strongly suggests that water organisation in micro-pores is not equivalent to that of bulk water. Superimposed protein layers of Type I and IV collagen, Type I collagen-fibronectin, Type I collagen-heparin, and Type I collagen-chondroitin sulphate increased diffusional resistance, but with disproportional retardation of ascorbate diffusion due to charge repulsion at collagen-heparin and collagen-chondroitin sulphate combinations. Diffusive resistance at natural tendon and cartilage was considerably smaller; diffusion coefficients ranged from 8.33 x 10(-6) to 1.09 x 10(-8) cm(2) s(-1).

Contributions in Obesity Surgery

by Christine Stroh, Member EUAS

Short Biography

Prof. Dr. med. habil. Christine Stroh
SRH Wald-Klinikum Gera GmbH - Germany

professional education:

Sep. 1987 – Aug. 1988	*Presemester at the county hospital, Gera (Germany)*
Sep. 1988 – Sep. 1994	*Medical school Friedrich-Schiller-University, Jena (Germany)*
Oct. 1994 – Mar. 1995	*Junior doctor: surgical ward, hospital Gera (Germany)*
Apr. 1995 – Mar. 1996	*Junior doctor: children surgery, FSU Jena*
Apr. 1996 – Jun. 2005	*Assistant doctor at the surgery hospital Gera, Germany Department of General, Visceral and Pediatric Surgery*
Feb. 2001	*Medical exermination for surgery*
since July 2005	*Senior physician: surgical center "SRH Wald-Klinikum Gera", Department of General, Visceral and Pediatric Surgery*
Jan. 2006	*Medical exermination for visceral surgery*
Sep. 2006	*Acquisition of additional qualification proctology*
Nov. 2007	*Acquisition of additional qualification nutritional medicine*
Aug. 2008 – Jul. 2011	*Sitting on classes in the department of general, visceral and pediatric surgery at the „Otto-von-Guericke" University, Magdeburg*
Jun. 2011	*Habilitation and attainment of Venia legendi at the "Otto-von-Guericke" University, Magdeburg*
Mar. 2016	*APL Professur of Surgery at the "Otto-von-Guericke" University, Magdeburg*

Professional knowledge:
Knowledge radiation protection
Knowledge in adiposity surgery
Knowledge in ultrasound
Knowledge in transrectal endosonography
Knowledge in anal manometry

Staple Line Leak After Primary Sleeve Gastrectomy-Risk Factors and Mid-term Results: Do Patients Still Benefit from the Weight Loss Procedure?

Benedix F, Poranzke O, Adolf D, Wolff S, Lippert H, Arend J, Manger T, **Stroh C**; Obesity Surgery Working Group Competence Network Obesity.
Obes Surg. 2017 Jul;27(7):1780-1788. doi: 10.1007/s11695-017-2543-7.

BACKGROUND
Staple line leak after laparoscopic sleeve gastrectomy (LSG) still represents the most feared complication. The purpose of this study was to investigate whether there are factors that increase the risk for a leakage. Furthermore, we aimed to analyze the impact of a leak on weight change and resolution of comorbidities.
METHODS
Since 2005, data from obese patients that undergo bariatric procedures in Germany are prospectively registered. For the current analysis, all adult subjects that had undergone primary LSG from 2005 to 2014 were considered.

RESULTS
Overall, 241/15,756 (1.53%) patients experienced a leak. The occurrence of a leakage resulted in a significant increase of the mortality rate (3.7 vs. 0.2%; $p < 0.01$). Percent excess weight loss did not differ between leak and non-leak patients, both, at 12 (64.2 vs. 60.9%; $p = 1.0$) and 24 months (68.5 vs. 64.0%, $p = 0.86$). Similarly, no significant difference was observed for resolution rate of all comorbid conditions. Matched pair analysis confirmed these findings. Multivariable analysis identified operation time, conversion, intraoperative complications, and hypertension and degenerative joint disease as risk factors for a leak. Oversewing the staple line was associated with the lowest risk.
CONCLUSION
The postoperative staple line leak after primary LSG significantly increases postoperative morbidity and mortality. We found that there are patient-related factors and operative variables that predispose to leakage after LSG. However, the occurrence of a leakage does not adversely impact the weight loss and resolution of comorbidities in the mid-term.

Risk of thrombosis and thromboembolic prophylaxis in obesity surgery: data analysis from the German Bariatric Surgery Registry.

Stroh C, Michel N, Luderer D, Wolff S, Lange V, Köckerling F, Knoll C, Manger T; Obesity Surgery Working; Group, Competence Network Obesity.
Obes Surg. 2016 Nov;26(11):2562-2571.

BACKGROUND
Evidence-based data on optimal approach for prophylaxis of deep venous thrombosis (VTE) and pulmonary embolism (PE) in bariatric operations is discussed. Using antithrombotic prophylaxis, weight adjusted the risk of VTE and its complications have to be balanced with the increased bleeding risk.
METHODS
Since 2005, the current situation for bariatric surgery has been examined by quality assurance study in Germany. As a prospective multicenter observational study, data on the type, regimen, and time course of VTE prophylaxis were documented. The incidences of clinically diagnosed VTE or PE were derived during the in-hospital course and follow up.
RESULTS
Overall, 31,668 primary bariatric procedures were performed between January 2005 and December 2013. Most performed operations were 3999 gastric banding (GB); 13,722 Roux-en-Y-gastric bypass (RYGBP); and 11,840 sleeve gastrectomies (SG). Gender ($p = 0.945$), surgical procedure ($p = 0.666$), or administration of thromboembolic prophylaxis ($p = 0.272$) had no statistical impact on the DVT incidence. By contrast, BMI ($p = 0.116$) and the duration of thromboembolic prophylaxis ($p = 0.127$) did impact the frequency of onset of DVT.
CONCLUSION
Age, BMI, male gender, and a previous history of VTE are the most important risk factors. The drug of choice for VTE is heparin. LMWH should be given preference over unfractionated heparins due to their improved pharmacological properties, i.e., better bioavailability and longer half-life as well as ease of use. Despite the low incidence of VTE and PE, there is a lack of evidence. Therefore, prospective randomized studies are necessary to determine the optimal VTE prophylaxis for bariatric surgical patients.

Closed-loop gastric electrical stimulation versus laparoscopic adjustable gastric band for the treatment of obesity: a randomized 12-month multicenter study.

Horbach T, Meyer G, Morales-Conde S, Alarcón I, Favretti F, Anselmino M, Rovera GM, Dargent J, **Stroh C**, Susewind M, Torres AJ.
Int J Obes (Lond). 2016 Dec;40(12):1891-1898. doi: 10.1038/ijo.2016.159. Epub 2016 Sep 16.

OBJECTIVE
To compare the weight loss, change in quality of life (QOL) and safety of closed-loop gastric electrical stimulation (CLGES) versus adjustable gastric band (LAGB) in the treatment of obesity.
METHODS
This multicenter, randomized, non-inferiority trial randomly assigned the patients in a 2:1 ratio to laparoscopic CLGES versus LAGB and followed them for 1 year. We enrolled 210 patients, of whom 50 were withdrawn preoperatively. Among 160 remaining patients (mean age=39±11 years; 75% women; mean body mass index=43±6 kg m^{-2}) 106 received CLGES and 54 received LAGB. The first primary end point was non-inferiority of CLGES versus LAGB, ascertained by the proportion of patients who, at 1 year, fulfilled: (a) a 20% excess weight loss (EWL); (b) no major device- or procedure-related adverse event (AE); and (c) no major, adverse change in QOL. Furthermore, 50% of patients had to reach 25% EWL. The incidence and seriousness of all AE were analyzed and compared using Mann-Whitney's U-test.
RESULTS
At 1 year, the proportions of patients who reached all components of the primary study end point were 66.7 and 73.0% for the LAGB and CLGES group, respectively, with a difference of -6.3% and an upper 95% CI of 7.2%, less than the predetermined 10% margin for confirming the non-inferiority of CLGES. The second primary end point was also met, as 61.3% of patients in the CLGES group reached 25% EWL (lower 95% CI=52.0%; P<0.01). QOL improved significantly and similarly in both groups. AE were significantly fewer and less severe in the CLGES than in the LAGB group (P<0.001).
CONCLUSIONS AND RELEVANCE
This randomized study confirmed the non-inferiority of CLGES compared with LAGB based on the predetermined composite end point. CLGES was associated with significantly fewer major AE.

Does Certification as Bariatric Surgery Center and Volume Influence the Outcome in RYGB-Data Analysis of German Bariatric Surgery Registry.

Stroh C, Köckerling F, Lange V, Wolff S, Knoll C, Bruns C, Manger T; Obesity Surgery Working Group, Competence Network Obesity.
Obes Surg. 2017 Feb;27(2):445-453. doi: 10.1007/s11695-016-2340-8.

AIM
To examine the association between the certification as bariatric surgery center and volume and patient outcome, data collected in the German Bariatric Surgery Registry were evaluated. All data were registered prospectively in cooperation with the Institute of Quality Assurance in Surgery at Otto-von-Guericke University Magdeburg.
METHODS
Data collection began in 2005 for all bariatric procedures in an online database. Participation in the quality assurance study is required for all certified bariatric surgery centers in Germany. Descriptive evaluation and matched pairs analysis were performed. Patients were matched via propensity score taking into account BMI, age, and incidence of comorbidities.
RESULTS
During the period from 2005 to 2013, 3083 male and 10,639 female patients were operated on with the RYGB primary approach. In Centers of Competence (77.2 %) and non-accredited hospitals (76.3 %), the proportion of female patients was significantly lower than in Centers of Reference/Excellence (78.7 %; $p = 0.002$). The mean age in Centers of Reference/Excellence (41.2 years) was significantly lower than in Centers of Competence (43.2 years; $p < 0.05$). Propensity score analysis was performed to compare matched patients with regard to BMI, age, and incidence of comorbidities. The rate of general and surgical postoperative complications and mortality rate was significantly lower in certified Centers of Reference/Excellence compared to Centers of Competence with 29 and non-certified hospitals.

CONCLUSION
There is evidence of improved patient outcome in certified bariatric surgery centers with higher volume. The study supports the concept of certification. There are different factors which can and cannot be preoperatively modified and influence the perioperative outcome.

Nutritional deficiencies and supplementation after metabolic surgery.

Stroh C, Meyer F, Manger T.
Chirurg. 2016 Sep;87(9):762-767. doi: 10.1007/s00104-016-0198-x. German.
Increasing prevalence of morbid obesity in Germany is associated with an increasing number of bariatric surgical interventions.Based on the effectiveness of bariatric surgery with regard to a significant reduction of body weight and comorbidity as well as improvement of the quality of life compared with conservative measures, its value and impact has been substantially increased. Long-term metabolic deficits such as nutrient deficiencies can be considered the main risks of various restrictive, combined and malabsorptive procedures of bariatric surgery.The aim of this overview is to characterize metabolic complications after bariatric surgery and their prophylaxis, which require a temporary or permanent surveillance and, if necessary, effective supplementation.Bariatric surgical interventions such as gastric banding (GB) and sleeve gastrectomy (SG) can be subsequently associated with deficiencies related to B-vitamins whereas iron, folate, and vitamins B1, B12 and D deficiencies might be consequences of malabsorptive procedures such as biliopancreatic diversion, duodenal switch and Roux-en-Y gastric bypass.Due to possible metabolic and surgical complications after bariatric surgery, patients need to undergo life-long follow-up investigations. The currently available guidelines of the American Association of Bariatric and Metabolic Surgery are the basis for the latest recommendations on supplementation and treatment in bariatric surgery.

Results of More Than 11,800 Sleeve Gastrectomies: Data Analysis of the German Bariatric Surgery Registry.

Stroh C, Köckerling F, Volker L, Frank B, Stefanie W, Christian K, Christiane B, Thomas M; Obesity Surgery Working Group, Competence Network Obesity.
Ann Surg. 2016 May;263(5):949-55. doi: 10.1097/SLA.0000000000001559.
BACKGROUND
Laparoscopic sleeve gastrectomy (SG) is an upcoming procedure in bariatric surgery and is currently performed worldwide. Staple line leakage, as the most frequent and most feared complication, is still a major concern.
METHODS
Since 2005 data from patients undergoing bariatric procedures in Germany have been prospectively registered in an online database and analyzed. All patients who had undergone primary SG within a 7-year period were considered for analysis.
RESULTS
Using the German Bariatric Surgery Registry, data from more than 11,800 SGs were collected between January 1, 2005, and December 31, 2013. Staple line leak rate decreased from 6.5% to 1.4%. Male sex, higher body mass index, concomitant sleep apnea, conversion to laparotomy, longer operation time, a combination of buttresses and oversewing, and the occurrence of intraoperative complications were associated with a significantly higher leakage rate compared with when using either buttresses or oversewing alone. On multivariable analysis, operation time and year of procedure only had a significant impact on staple line leakage rate.

Materials Science, Novel Materials for Energy Storage and Conversion

by Meilin Liu, Member EUAS

Short Biography

Meilin Liu is the B. Mifflin Hood Chair Professor, Regents' Professor, and Associate Chair in the School of Materials Science and Engineering at Georgia Institute of Technology, Atlanta, Georgia, USA. He received his B.S. from South China University of Technology and his M.S. and Ph.D. from the University of California at Berkeley. (http://fcbt.mse.gatech.edu/Mliu.html)

He is known for his investigations into the mechanisms of electrode reactions associated with chemical and energy transformation processes, especially in simultaneously performing Raman spectroscopy and electrochemical measurements in order to gain critical insights into the mechanisms of charge & mass transfer along surfaces and across interfaces in porous electrodes. His work is vital to unraveling the science of electrode processes and to providing scientific basis for rational design of surfaces, interfaces, and porous electrodes for fuel cells, batteries, and supercapacitors. He has published more than 430 refereed journal papers, edited 7 books, and been awarded 27 US/World patents, with an h-index of 91 (Google Scholar). Currently, his research interests are focused on in-situ/operando characterization of surface and interfaces, and the development of novel materials inspired by Nature.

His outstanding contributions have been recognized by various awards and honors, including NSF National Young Investigator award (1993), Georgia Tech Outstanding Faculty Research Author award (twice in 1999 and 2013), Georgia Tech Outstanding Achievement in Research Program Development award (2003), Sigma Xi Sustained Research award (2003), American Ceramic Society Ross Coffin Purdy award for outstanding contribution to ceramics literature (2010), Fellow of American Ceramic Society (2011), Fellow of Electrochemical Society (2012), B. Mifflin Hood Chair Professorship (2015), Kolon Fellow (2017), and member of EUAS (2017).

The sustainable supply of clean and economical energy is a global challenge. The world is at a transition in the generation, storage, and the use of energy. New energy technologies must be developed to meet the ever-increasing demands for energy, which is expected to double over the next few decades. The next generation of energy technologies will profoundly influence the cars we drive, the air we breathe, and the way we live.

Of the energy we are using today, more than 82% is generated from fossil fuels (such as coal, petroleum, and natural gas) and about 8% from nuclear power using conventional technologies; only about 10% is derived from renewable sources such as hydroelectric, biomass, solar, and other sources. The energy efficiency of conventional technologies is relatively low, especially in the transportation sector, where the overall efficiency is only about 20%, implying that about 80% of the energy used in transportation is lost as rejected heat or through other inefficiencies. It is indisputable that we can no longer use fossil fuels in a conventional way; it is not only unsustainable and unable to meet the future demands (due to limited resources) but also unacceptable because of the unbearable environmental consequences.

Clearly, the only viable solution is that we must use alternative energy derived from renewable natural resources that do not harm the environment such as hydroelectric, solar, wind, biomass, ocean/tides, and geothermal energy. This energy is sustainable because its use today does not compromise the ability to meet the needs in the future. To date, unfortunately, the primary limiting factors for broad commercialization of alternative

energy technologies is their low efficiency and poor economic competitiveness. To significantly enhance the performance while reducing the cost, it is imperative to gain fundamental understanding of the mechanisms of energy and chemical transformation processes and, thus, to achieve rational design of novel materials with dramatically higher levels of functionalities and performance. Transformational scientific breakthroughs are urgently needed to meet the enormous energy challenges.

The objective of Dr. Liu's research is to tackle the grand energy challenges. His team is focusing on fundamental research that will lead to scientific breakthroughs for producing, storing, and using energy. The goal is to create transformational technologies that will enable us to cost-effectively generate electricity from renewable sources and power our vehicles by a new generation of batteries and fuel cells.

Since materials play a vital role in efficient and cost effective utilization of energy, the focus of Dr. Liu's research is centered on the development of novel materials with chemistries, structures, morphology, and architecture tailored for dramatic improvements in efficiencies for chemical and energy transformation. Many unique nanostructured materials are being explored for energy storage and conversion, including nano-particles, -wires, -tubes, -belts, -sheets, and intricate 3-dimensional nano-porous assemblies of different types of materials. Fundamentally new protocols are being developed to control the materials' structures over multiple length scales to allow for a new generation of hierarchical materials with more accessible surfaces, higher functionalities, and shorter diffusion distances for greatly enhanced rate capabilities.

Dr. Liu is an internationally renowned leader in solid oxide fuel cells (SOFCs) and advanced materials for electrochemical energy storage and conversion. He has built a world-class program at Georgia Tech on synthesis, fabrication, modeling, and *in situ/operando* characterization of membranes, thin films, and porous electrodes for energy storage and conversion, aiming to achieve rational design of novel materials and structures with unique functionalities. His research has been supported by various federal agencies, national labs, and about 30 companies. His group has developed unique approaches to probing/mapping electrode reactions under *in situ/operando* conditions, providing critical insight into the mechanisms of ionic transport and electrochemical processes occurring on surfaces and across interfaces. His research has influenced the understanding and rational design of novel materials and structures as well as practical concepts for fuel cells, batteries, and sensors.

He has edited 7 books, authored/co-authored ~ 430 refereed articles, 12 invited reviews, and 7 book chapters, and presented ~180 invited talks, of which many are keynote/plenary lectures. His work is published in highly reputed journals such as *Science (1), Nature (1), Nature Comms (3), Energy Environ. Sci. (12), Adv. Mater. (15), Adv. Energy Mater.(15), Chem. Soc. Rev (1), Nano Letters (7), Angew. Chem. Int. Ed. (6), JACS (2), MSE Report (2), Progress in Mat. Sci. (1), Adv. Functional Mater.(6), Nano Energy (16)*, and so forth.

The worldwide recognition of his distinctive and significant contributions to the profession is evident from his invitations to give many talks at major national and international meetings and by his significant publications in the literature (Google Scholar citations>28,500, h-index: 91). The impact of his research is evident by his being awarded ~$21M in contracts, grants, and gifts to support his research and being the inventor/co-inventor of 27 US/world patents on new concepts, novel materials, and unique devices.

Some of his most notable contributions are briefly summarized as follows:

- Developed a new class of mixed-ion conductors, $BaZr_{0.1}Ce_{0.7}Y_{0.2-x}Yb_xO_{3-d}$, with the highest proton conductivities at intermediate temperatures and remarkable tolerance to sulfur poisoning under conditions for fuel cell operation, reforming, and H_2 production;[1]
- Developed nanostructured BaO/Ni anode that efficiently oxidizes fuel with minimum carbon build-up, making it possible for most efficient conversion to electricity of readily available fuels (e.g., natural gas and coal gas);[2]
- Advanced Raman spectroscopic techniques for *in situ/operando* characterization of electrode surfaces;[3-8]
- Designed and implemented catalyst-coated SOFC cathodes with dramatically enhanced ORR activity and durability;[9-11]
- Designed and fabricated durable fiber-based SOFC cathodes, [12-13] electro-catalysts for efficient water splitting,[14-16] and high energy & power density electrodes for supercapacitors. [17-19]
- Applied a "shape-preserving" conversion process for preparation of complex porous electrodes using biogenic templates with variety of 3D micro- to nano-scale features[20] and demonstrated superior performance of electrodes derived from complex templates;[21]
- Developed a process for electro-deposition of 3D porous electrodes,[22-24] a low-cost combustion CVD process for fabrication of thin films, nanoparticles, nanotubes, and nanostructured electrodes[25-26] with great flexibility in composition and microstructure;
- Developed triazole-based polymer electrolytes of high proton conductivity at high temperatures with little dependence on humidity,[27-29]
- Developed a class of disulfide polymerization electrodes for Li-batteries,[30-31] leading to the founding of PolyPlus Battery Company focusing on advanced Li battery technology.

Dr. Liu is also an effective educator and mentor. To date, he has supervised 33 postdoctoral fellows, 29 visiting scholars, 35 PhD students, 25 joint PhD students, 13 MS students, and numerous undergraduate researchers. More than 20 of his former students are now conducting pioneering research as faculty members at universities in the U.S., China, South Korea, and Spain, while many others are research scientists in major industrial research centers (e.g., GE, United Technologies. Air Products, BASF, Apple, and Phillips 66).

References

1. L. Yang, S. Wang, K. Blinn, M.F. Liu, Z. Liu, Z. Cheng, M. Liu, Enhanced Sulfur and Coking Tolerance of a Mixed Ion Conductor for SOFCs: BZCYYb, ***Science***, **326**, 126-129, 2009.
2. L. Yang, Y. Choi, W. Qin, H. Chen, K. Blinn, M. F. Liu, P. Liu, J. Bai, T. A. Tyson, M. Liu, Promotion of Water-Mediated Carbon Removal by Nanostructured BaO/Ni Interfaces in Solid Oxide Fuel Cells, ***Nature Communications***, 2, 357, (2011).
3. D.C. Chen, J. H. Wang, T. F. Chou, B. Zhao, M.A. El-Sayed, M. Liu, "Unraveling the nature of anomalously fast energy storage in T-Nb_2O_5, ***J. Am. Chem. Soc.,*** 139, 7071 (2017).
4. X. Li, J. Lee, K. Blinn, D. Chen, S. Yoo, B. Kang, L. Bottomley, M. El-Sayed, S. Park, M. Liu, High-temperature surface enhanced Raman spectroscopy for in situ study of solid oxide fuel cell materials ***Energy Environ. Sci***., 2014, 7, 306.
5. X. Li, M. F. Liu, J. P. Lee, D. Ding, L. A. Bottomley, S. Park, M. Liu, An operando surface enhanced Raman spectroscopy (SERS) study of carbon deposition on SOFC anodes ,***Phys. Chem. Chem. Phys.***, 2015, 17, 21112 | DOI: 10.1039/C4CP05176A
6. D. Chen, X. Xiong, B. Zhao, M. Mahmoud, M. A. El-Sayed, M. Liu, Probing Structural Evolution and Charge Storage Mechanism of NiO_2H_x Electrode Materials using In Operando Resonance Raman Spectroscopy, ***Advanced Science,*** 2016, 1500433. DOI: 10.1002/advs.201500433
7. D. Chen, D. Ding, X. Li, G. Waller, X. Xiong, M. El-Sayed, M. Liu,Probing the charge storage mechanism of a pseudocapacitive MnO_2 electrode using in operando Raman spectroscopy, ***Chem. Mater.***, 2015, 27, 822-828 | DOI: 10.1021/acs.chemmater.5b03118
8. Z. Cheng, J. H. Wang, Y. M. Choi, L. Yang, M. C. Lin, M. Liu, From Ni-YSZ to Sulfur-Tolerant Anodes: Electrochemical Behavior, Modeling, In Situ Characterization, and Perspectives, ***Energy & Env. Sci***., **4**, 4380-4409,

2011.
9. Y. Chen, Y. Chen, D. Ding, Y. Ding, Y. Choi, L. Zhang, S. Yoo, D. Chen, B. deGlee, H. Xu, Q. Lu, B. Zhao, G. Vardar, J. Wang, H. Bluhm, E. Crumlin, C. Yang, J. Liu, B. Yildiz, M. Liu, A robust and active hybrid catalyst for facile oxygen reduction in solid oxide fuel cells, ***Energy Environ. Sci.***, 10, 964-971, 2017.
10. D. Ding, X. Li, S. Lai, K. Gerdes, M. Liu, Enhancing SOFC Cathode Performance by Surface Modification through Infiltration, ***Energy Environ. Sci.***, 2014, 7, 552-575.
11. Y. Li, J. Chen, Y. Zheng, B. Yu, Y. Chen, M. Liu, Controlling cation segregation in perovskite-based electrodes for high electro-catalytic activity and durability , ***Chemical Society Review*** , 2017, 46, 6345| DOI: 10.1039/C7CS00120G
12. Yu Chen, Yunfei Bu, Yanxiang Zhang, Ruiqiang Yan, Dong Ding, Bote Zhao, Seonyoung Yoo, Dai Dang, Renzong Hu, Chenghao Yang, and M. Liu, A Highly Efficient and Robust Nanofiber Cathode for Solid Oxide Fuel Cells, ***Advanced Energy Materials*** , 2017, 7, 1601890 | DOI: 10.1002/aenm.201601890
13. Yu Chen, Yunfei Bu, Bote Zhao, Yanxiang Zhang, Dong Ding, Renzong Hu, Tao Wei, Ben Rainwater, Yong Ding, Fanglin Chen, Chenghao Yang, Jiang Liu, Meilin Liu, A durable, high-performance hollow-nanofiber cathode for intermediate-temperature fuel cells, ***Nano Energy***, 26 (2016): 90-99.
14. B. Zhao, L. Zhang, D. Zhen, S. Yoo, Y. Ding, D. Chen, Y. Chen, Q. Zhang, B. Doyle, X. Xiong, M. Liu, A tailored double perovskite nanofiber catalyst enables ultrafast oxygen evolution, ***Nature Communications*****,** 8, 14586 (2017).
15. Y. Zhu, W. Zhou, Y. Chen, J. Yu, M. Liu, Z. Shao, A High-Performance Electrocatalyst for Oxygen Evolution Reaction: $LiCo_{0.8}Fe_{0.2}O_2$, ***Advanced Materials***, 27, 7150 (2015).
16. Y. Zhu, W. Zhou, Y. Zhong, Y. Bu, X. Chen, Q. Zhong, M. Liu, Z. Shao, A Perovskite Nanorod as Bifunctional Electrocatalyst for Overall Water Splitting", ***Advanced Energy Materials***, 2017, 7, 1602122 | DOI: 10.1002/aenm.201602122.
17. L. Huang, D. Chen, Y. Ding, S. Feng, Z. Wang, M. Liu, Nickel-cobalt hydroxides nanosheets coated on $NiCo_2O_4$ nanowires grown on carbon fiber paper for high-performance pseudocapacitors, ***Nano Letters*****,** 2013, 13 (7), pp 3135-3139. dx.doi.org/10.1021/nl401086t
18. B. Zhao, D. Chen, X. Xiong, B. Song, R. Hu, Q. Zhang, B. Rainwater, G. Waller, D. Zhen, Y. Ding, Y. Chen, C. Qu, D. Dang, C. P. Wong, M. Liu, A high-energy, long cycle-life hybrid supercapacitor based on graphene composite electrodes, ***Energy Storage Materials*****,** 7 (2017) 32-39 | http://dx.doi.org/10.1016/j.ensm.2016.11.010
19. M. K. Song, S. Cheng, H. Chen, W. Qin, J. Bai, T. Tyson, Nan, Yang, S. Xu, A. Bongiorno, & M. Liu, Anomalous Pseudocapacitive Behavior of a Nanostructured, Mixed-Valent Manganese Oxide Film for Electrical Energy Storage, ***Nano Letters***, 12(6) 3483-3490, 2012, DOI:10.1021/nl300984y.
20. Z. Bao, M. Weatherspoon, Y. Cai, S. Shian, G. Ahmad, M. Dickerson, B. Church, Z. Kang, H. Abernathy, C. Summers, M. Liu, K. Sandhage, Chemical Reduction of Three-Dimensional Silica Micro-Assemblies into Microporous Silicon Replicas, ***Nature*****,** 446(7132), 172-175, 2007.
21. Z. Bao, M. Song, S. Davis, Y. Cai, M. Liu, K. Sandhage, Shape-preserving Reactive Conversion of Complex-shaped 3D Silica Micro-assemblies into High Surface Area Micro/mesoporous Carbon and Platinum-loaded Carbon, ***Energy Environ. Sci.***, 2011, 4, 3980-3984.
22. H. C. Shin, J. Dong, and M. Liu, Nanoporous Structures Prepared by an Electrochemical Deposition Process, ***Advanced Materials***, **15** (19), 1610-1614, 2003.
23. H. C. Shin, J. Dong, and Meilin Liu, Porous Tin Oxides Prepared Using an Anodic Oxidation Process, ***Advanced Materials***, 16(3), 237-240, 2004.
24. H. C. Shin, Meilin Liu, Three-Dimensional Porous Copper-Tin Alloy Electrodes for Rechargeable Lithium Batteries, ***Advanced Functional Materials***, 5(4), 582-586, 2005.
25. Y. Liu, J. Dong, and Meilin Liu, Well Aligned Nano- 'Box Beams' of SnO_2, ***Advanced Materials***, 16 (4), 353-356, 2004.
26. Y. Liu, S. Zha, and Meilin Liu, Novel Nanostructured Electrodes Fabricated by Combustion CVD, ***Advanced Materials***, 16 (3) 256-260, 2004.
27. M. Song, H. Li, J. Li, D. Zhao, J. Wang, M. Liu, Tetrazole-based, Anhydrous Proton Exchange Membranes for Fuel Cells, ***Advanced Materials*****,** 2014, 26, 1277-1282. | DOI: 10.1002/adma.201304121
28. Z. Zhou, S. Li, Y. Zhang, M. Liu, W. Li, Promotion of Proton Conduction in Polymer Electrolyte Membranes by 1H-1,2,3-Triazole, ***J. Am. Chem. Soc***., 127, 10824, 2005. (also resulted in several US Patents)
29. M. Liu, X. Zhu, M. Song, J. Muldoon, K. Hase, Fuel cell electrodes with triazole modified polymers and MEA incorporating same, ***US Patent*** *9,012,108*, 4/21/2015
30. M. Liu, S. J. Visco, and L. C. De Jonghe, Novel Solid Redox Polymerization Electrodes for – All-Solid State, Thin-Film, Rechargeable Lithium Batteries, ***J. Electrochem. Soc***., **138**, 1891-1895, 1991. (also resulted in several US Patents)
31. M. Liu, S. J. Visco, and L. C. De Jonghe, Electrode Kinetics for Organo-disulfides Cathodes for Storage Batteries, ***J. Electrochem. Soc***.,137, 750-759, 1990.

New Contributions in Cardiovascular Medicine

by Hiroaki Shimokawa, Member EUAS

Short Biography

Dr. Shimokawa is Professor and the Chairman of the Department of Cardiovascular Medicine, Tohoku University Graduate School of Medicine, Sendai, Japan. Dr. Shimokawa graduated from Kyushu University in 1979, obtained PhD degree in 1985, and has been appointed for the present position in 2005.

His research projects include (1) molecular mechanisms of coronary artery spasm and atherosclerosis, (2) endothelial function, (3) development of innovative medical therapies, and (4) large clinical trials of heart failure and ischemic heart disease. He is well known for the development of animal models of coronary spasm (Science 1983) and the identification of endothelium-derived hydrogen peroxide as an important endothelium-derived relaxing factor (J Clin Invest 2000). He is also the pioneer for the development of extracorporeal cardiac shock wave therapy for the treatment of severe angina pectoris (Circulation 2004). He has published more than 500 peer-reviewed papers in the leading journals, such as Science, the Lancet, the Journal of Clinical Investigation, Circulation, the Journal of the American College of Cardiology, European Heart Journal, Circulation Research, and ATVB.

He received the Satoh Award (the Society Award) of the Japanese Circulation Society (JCS) in 1999, the Jeffrey M. Hoeg Award of the American Heart Association (AHA) in 2006, the Japan Medical Association Award in 2012, and the William Harvey Lecture Award of the European Society of Cardiology (ESC) in 2014.

He served as the Editor-in-Chief of Circulation Journal (JCS) for 8 years (2008-2016), and currently served as an Associate Editor of European Heart Journal (ESC) and ATVB (AHA) and a Senior Consulting Editor of Circulation Research (AHA), in addition to the editorial board members of many other international journals, including Circulation and American Journal of Physiology.

He also serves as the president of the Japanese Society for Gender-specific Medicine, the Nitric Oxide Society of Japan and the Japanese Pulmonary Circulation Society, in addition to the board members of the Japanese Circulation Society, the Japanese College of Cardiology, the Japanese Heart Failure Society, the Japanese Society for Cardiovascular Research, the Japanese College of Angiology, the Japanese Association of Cardiac rehabilitation, etc. He also is a Fellow of the American Heart Association (AHA) and the European Society of Cardiology (ESC).

Comprehensive evaluation of the effectiveness and safety of balloon pulmonary angioplasty for inoperable chronic thromboembolic pulmonary hypertension -Long-term effects and procedure-related complications.

Aoki T, Sugimura K, Tatebe S, Miura M, Yamamoto S, Yaoita N, Suzuki H, Sato H, Kozu K, Konno R, Miyata S, Nochioka K, Satoh K, **Shimokawa H.** ***Eur Heart J***. 38:3152-3159,2017

Aims

Although balloon pulmonary angioplasty (BPA) improves haemodynamics and short-term prognosis in patients with inoperable chronic thrombo-embolic pulmonary hypertension (CTEPH), the long-term effects of BPA, and procedure-related complications remain to be fully elucidated.

Methods and results

From July 2009 to October 2016, we performed a total of 424 BPA sessions in 84 consecutive patients with inoperable CTEPH. We used 3D reconstructed computed tomography to determine target lesions of pulmonary arteries and optical computed tomography to select balloon size, if needed. In 77 patients (92%) who completed the BPA treatment [65 ± 14 (SD) years-old, male/female 14/63], haemodynamics and exercise capacity were examined at 6 months after last BPA and in the chronic phase [>12 months after first BPA, 31 (20, 41) months]. The BPA treatment significantly improved mean pulmonary arterial pressure (38 ± 10 to 25 ± 6 mmHg), pulmonary vascular resistance (7.3 ± 3.2 to 3.8 ± 1.0 Wood units), and 6-minute walk distance (380 ± 138 to 486 ± 112 m) (all $P < 0.01$), and the improvements persisted throughout the follow-up period (43 ± 27 months) (N= 53). In the 424 sessions, haemoptysis was noted in 60 sessions (14%), and non-invasive positive pressure ventilation (NPPV) was used to treat haemoptysis and/or hypoxemia in 33 sessions (8%). Furthermore, 5-year survival was 98.4% (only one patient died of colon cancer) with no peri-procedural death.

Conclusion

These results indicate that BPA improves haemodynamics and exercise capacity in inoperable CTEPH patients with acceptable complication rate and that the beneficial haemodynamic effects of BPA persist for years with resultant good long-term prognosis.

Age-specific trends in the incidence and in-hospital mortality of acute myocardial infarction over 30 years in Japan - Report from the Miyagi AMI Registry Study

Cui Y, Hao K, Takahashi J, Miyata S, Shindo T, Nishimiya K, Kikuchi Y, Tsuburaya R, Matsumoto Y, Ito K, Sakata Y, **Shimokawa H.** ***Circ J***. 81:520-528,2017.

Background

We are now facing rapid population aging in Japan, which will affect the actual situation of cardiovascular diseases.However, age-specific trends in the incidence and mortality of acute myocardial infarction (AMI) in Japan remain to be elucidated.

Methods and Results

We enrolled a total of 27,220 AMI patients (male/female 19,818/7,402) in our Miyagi AMI Registry during the past 30 years. We divided them into 4 age groups (≤59, 60–69, 70–79 and ≥
80 years) and examined the temporal trends in the incidence and in-hospital mortality of AMI during 3 decades (1985–1994, 1995–2004 and 2005–2014). Throughout the entire period, the incidence of AMI steadily increased in the younger group (≤59 years in both sexes), while in the elderly groups (≥70 years in both sexes), the incidence significantly decreased during the last decade (all $P<0.01$). In-hospital cardiac mortality significantly decreased during the first 2 decades in elderly groups of both sexes (all $P<0.01$), whereas no further improvement was noted in the last decade irrespective of age or sex, despite improved critical care of AMI.

Conclusions

These results provide the novel findings that the incidence of AMI has been increasing in younger populations and decreasing in the elderly, and that improvement in the in-hospital mortality of AMI may have reached a plateau in all age groups in Japan.

Coronary artery ectasia predicts future cardiac events in patients with acute myocardial infarction.

Doi T, Kataoka Y, Noguchi T, Shibata T, Nakashima T, Kawakami S, Nagai T, Kanaya T, Tahara Y, Asaumi Y, Tsuda E, Nakai M, Nishimura K, Anzai T, Kusano K, **Shimokawa H**, Goto Y, Yasuda S. ***Arterioscler Thromb Vasc Biol***. 37:2350-2355,2017.

Objective
Coronary artery ectasia (CAE) is an infrequently observed vascular phenotype characterized by abnormal vessel dilatation and disturbed coronary flow, which potentially promote hrombogenicity and inflammatory reactions. However, whether or not CAE influences cardiovascular outcomes remains unknown.
Approach and Results
We investigated major adverse cardiac events (MACE; defined as cardiac death and nonfatal myocardial infarction [MI]) in 1698 patients with acute MI. The occurrence of MACE was compared in patients with and without CAE. CAE was identified in 3.0% of study subjects. During the 49-month observation period, CAE was associated with 3.25-, 2.71-, and 4.92-fold greater likelihoods of experiencing MACE (95% confidence interval [CI], 1.88–5.66; P<0.001), cardiac death (95% CI, 1.37–5.37; P=0.004), and nonfatal MI (95% CI, 2.20–11.0; P
<0.001), respectively. These cardiac risks of CAE were consistently observed in a multivariate Cox proportional hazards model (MACE: hazard ratio, 4.94; 95% CI, 2.36–10.4; P<0.001) and in a propensity score–matched cohort (MACE: hazard ratio, 8.98; 95% CI, 1.14–71.0; P=0.03). Despite having a higher risk of CAE-related cardiac events, patients with CAE receiving anticoagulation therapy who achieved an optimal percent time in target therapeutic range, defined as ≥ 60%, did not experience the occurrence of MACE (P=0.03 versus patients with percent time in target therapeutic range <60% or without anticoagulation therapy).
Conclusions
The presence of CAE predicted future cardiac events in patients with acute MI. Our findings suggest that acute MI patients with CAE are a high-risk subset who might benefit from a pharmacological approach to controlling the coagulation cascade.

Development of a novel shock wave catheter ablation system -A validation study in pigs in vivo

Hirano M, Yamamoto H, Hasebe Y, Fukuda K, Morosawa S, Amamizu H, Ohyama K, Uzuka H, Takayama K, **Shimokawa H**. ***Europace***. doi: 10.1093/europace/eux244

Aims
Although the radiofrequency catheter ablation (RFCA) is widely used for the treatment of tachyarrhythmias, it has three fundamental weaknesses as a thermal ablation system, including a limited lesion depth, myoendocardial injury linking to thromboembolism, and prolonged inflammation followed by subsequent recurrences. In order to overcome these limitations, we have been developing a shock wave (SW) catheter ablation (SWCA) system as a novel non-thermal therapy. In the present study, we validated our new SWCA system with increased SW intensity.

Methods and results

In a total of 36 pigs, we applied our new SWCA to ventricular muscle in vivo for the following protocols. (i) Epicardial approach (n= 17): The lesion depth achieved by the SWCA from the epicardium was examined. High intensity SW achieved 5.2 ± 0.9 mm lesions (35 applications), where there was a strong correlation between SW intensity and lesion depth (R= 0.80, P< 0.001, 54 applications). (ii) Endocardial approach (n= 6): The extent of endocardial injury with the two energy sources was examined by electron microscopy (8 applications each). Shock wave catheter ablation markedly reduced myoendothelial injury compared with RFCA (4.3 ± 1.2 vs. 79.6 ± 4.8%, P< 0.01). The electrophysiological effects on the SW lesions were also confirmed using three-dimensional mapping system. (iii) Time-course study (n= 6 each): The healing process after ablation therapy was examined. We found transient inflammatory responses and accelerated reparative process with preserved blood flow in the SWCA group.

Conclusion

These results indicate that our SWCA system is characterized, as compared with RFCA, by deeper lesion depth, markedly less myoendocardial injury and accelerated tissue repair process.

Innovative Aspects in Biochemistry

by Etana Padan

Short Biography

ACADEMIC TRAINING

1958-1963 *Received M.Sc. degree with honors, Major subject: Biochemistry. Minor subject: Physiology and Genetics.*

1963-1969 *Received Ph.D. degree, Ph.D. Thesis: Study of the Properties of Blue-Green Algal Viruses." Worked under the guidance of Prof. M. Shilo, Department of Microbiological Chemistry. Hebrew University Hadassah Medical School.*

PROFESSIONAL EXPERIENCE

1969 *Appointed Instructor in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.*

1970 *Appointed Research Fellow (Lecturer) in the Department of Microbiological Chemistry, Hebrew University-Hadassah Medical School.*

1972 *Research Fellow in the Department of Biochemistry, Weizmann Institute, Rechovot. (Post Doctorate with Prof. M. Avron and Prof. H. Rottenberg).*

1973 *Visiting Fellow in the Department of Zoology, Rand Afrikaans University, Johannesburg, Republic of South Africa.*

1974 *Appointed Senior Lecturer in the Department of Microbiological Chemistry, Hebrew University.*

1977 *Received tenure (Senior Lecturer).*

1978-1979 *Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.*

1979 *Appointed Associate Professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*

1980 *Appointed the head of the Oceanography programme in the Hebrew University.*

1982 *Appointed a science advisor in Biochemistry by the Binational Science Foundation.*

1983 *Member of the organizing committee of the 2nd International Workshop on primary productivity held in April, 1984, Haifa, Israel.*

1985 *Appointed full professor in the Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*

1985-1986 *Visiting scientist (Sabbatical) in the Department of H.R. Kaback, Membrane Biochemistry, Roche Institute of Molecular Biology, Nutley, New Jersey, U.S.A.*
Member of the Editorial Board of FEMS Microbiology Reviews.

1988 *Member of the organizing committee of the 6th International Symposium on Photosynthetic Prokaryotes, Holland, August, 1988.*

1989 *Head of Department of Microbial and Molecular Ecology, Life Sciences Institute, Hebrew University, Jerusalem.*

1990 *Visiting Professor in the Department of Biochemistry, Mount Sinai Medical Center of the University of New York.*

1992-1995 *Head of Institute of Life Sciences, Hebrew University of Jerusalem, October, 1992.*

1995 *Awarded M. Launda Prize of the Israeli Payis Institute for "Understanding of Physiology of Microorganisms and Their Adaptations to Changing Environment."*

1996 *Awarded EMBO Fellowship, Visiting Professor with Prof. H. Michel, Max-Planck-Institute fur Biophysik, Frankfurt, Germany.*

1998 *Chairperson of The Second FISEB, Societie of Experimental Biology, Eilat December, 1998.*

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

Na^+/H^+ antiporters are critical to homeostatic processes that regulate intracellular pH, Na^+ content, and volume (see recent reviews in [1; 2]). These antiporters are present in cells' cytoplasmic and organelle membranes [3] and are important drug targets [4; 5].

Ec-NhaA (herein NhaA), the principal Na^+/H^+ antiporter of *Escherichia coli*, is the most intensively studied Na^+/H^+ antiporter. NhaA enables *E. coli* cells to adapt to conditions of high salinity and to grow at alkaline pH (in the presence of Na^+ [6]), as well as to avoid toxic effects in the presence of high concentrations of Li^+. Homologues of NhaA are highly prevalent among enterobacteria [7], and the antiporter has orthologues throughout the biological kingdoms, including in humen [8].

NhaA catalyzes coupled stoichiometric antiport of $2H^+$ and $1Na^+$ across the membrane, with very high turnover [9; 10]. Its function is heavily dependent on pH [9], a property NhaA shares with other prokaryotic [6] and eukaryotic Na^+/H^+ antiporters (reviewed in [3; 4; 11; 12; 13]).

Initial insights regarding Na^+/H^+ antiporters mechanism of antiport and pH regulation [14] have been obtained from the crystal structure (Fig. 1) of down-regulated NhaA crystallized at acidic pH [15], a collaboration between Padan's group and the group of Hartmut Michel (Max-Planck Institute of Biophysics, Frankfurt, Germany). Very similar crystal structure has again been described at acidic pH with a difference in the position of TM (trans membrane segment) X [16]. It is still not known whether the reason for the difference between the two structures is a wrong helix assignment in the original structure or that the two structures represent different conformations. As yet neither the active conformations of NhaA at alkaline pH nor the bound ligands (Na^+/Li^+) have been determined. Therefore, our collaboration focuses now on determining the structure of active NhaA with bound Na^+/Li^+ at alkaline pH using all state of art techniques. These include for example, the LCP (Lipidic Cubic Phase) technique, test of new detergents and fixing the NhaA

conformations by fragments of monoclonal antibodies [17] and nanobodies which we have already produced.

Nevertheless, the acidic pH NhaA crystal structure has provided key insight into the function and regulatory properties of the antiporter, shaded new light on the general architecture of transport proteins and opened the way to structure based interdisciplinary studies of the Na^+/H^+ antiporters that could not otherwise have been carried out, as described below.

1. *Structural insights*: NhaA is a dimer and its monomer consists of 12 TMs (Fig. 1, TMs I-XII). The TMs of each monomer are assembled in two domains: the first domain is the interface domain that connects the two monomers into a dimer, and the second is the core domain (Fig. 1). The two domains encompass a large cytoplasmic funnel (lined by TMs II, IVc, V and IX) and a shallow periplasmic funnel (lined by TMs II, VIII and XIp (Fig. 1)). A hydrophobic barrier separates the two funnels [15].

The NhaA structure revealed in the core domain (TMs III, IV, V, X, XI, XII) a previously unknown fold (the NhaA fold) [18] in which TMs III, IV, V are topologically inverted with respect to TMs X, XI and XII. In each repeat, one TM (IV and XI, respectively) is interrupted by an extended chain that crosses the other in the middle of the membrane, creating two sets of small helices, one facing the cytoplasm (TM IVc and TM XIc), and one facing the periplasm (TM IVp and TM XIp) (Fig. 1). The crossing results in an environment in the middle of the membrane which is very delicately balanced electrostatically. Remarkably, structures of several other bacterial ion-coupled secondary transporters, which share little or no DNA sequence homology with NhaA, have been shown to possess the NhaA structural fold [19; 20; 21; 22].

What are the roles of the NhaA unique structural fold? Is it important for stability or has it also a functional role in the antiporter mechanism and its regulation? Answering these questions is the other main goal of Padan's group.

2. *Functional insights*: NhaA is a canonical secondary transporter, a "nano- machine" that alternates its active site between one side of the membrane and the other [23; 24]. As such, it is highly dynamic and changes conformation during activity and pH regulation. To understand this dynamic mechanism we are using structure-based approaches, combining computation, structural biology, biochemistry, biophysics and molecular biology to gain the following insights: a) The functional organization of NhaA. Cys scanning and site specific mutagenesis of many residues along NhaA is followed by characterization of the mutants' salt resistance-growth and antiporter activity in isolated membrane vesicles and/or pure protein reconstituted into proteoliposomes [2]. Using this procedure we have already identified two groups of amino acids; one group forms the NhaA active site, another cluster of amino acids participates in sensing environmental pH and controls the NhaA activity according to intracellular pH. b) Electrophysiology of NhaA, a collaboration between my group and the group of Klaus Fendler (Max Planck Institute of Biophysics, Frankfurt Germany). Electrophysiology is an established method to characterize eukaryotic transporters-functionality using voltage clamp or patch clamp methods. However, apart from few cases, bacterial transporters cannot be investigated with these techniques because of the small size of bacteria and because bacterial transporters are difficult to express in mammalian cells or oocytes. Electrophysiology based on solid supported membranes (SSM) has been found extremely useful for applying electrophysiology to bacterial transporters [25]; identifying electrogenic partial reactions, determine rate constants and substrate affinities and develop kinetic models for transport reactions. SSM based-electrophysiology has been applied to the study of the kinetic parameters of NhaA [26; 27; 28]. For the first time, forward and reversed transport reactions were investigated at zero membrane potential using right side out and inside-out membrane vesicles [27]. Although partial reactions of NhaA have not yet been identified, the electrophysiological results reveal that the Na^+/H^+ antiport activity is highly symmetrical and a kinetic model has been advanced in line with the alternating accessibility mechanism [27]; during ion translocation, Na^+ and H^+ compete at the active site. This competition has also been suggested to underlie the pH regulation of NhaA. However, experimental results as well as structural results (see below) imply that in addition to the exchange activity at the active site there is a pH sensor/transducer site that regulates the pH response of NhaA. c) pH- and substrate-induced site-specific conformational changes. This project involves introduction of site- specific reporters (tryptophan in a tryptophan-less background) into the protein

[29]. The reporters change signals upon addition of substrates or a pH shift and report upon conformational changes at specific sites in the protein. Two conformational changes were identified; Trp at position 136 specifically monitors a pH-induced conformational change that activates NhaA whereas a Trp at position 339 senses a ligand induced conformational change that does not occur until NhaA is activated at alkaline pH [29]. Another approach is testing accessibility of SH alkylating agents to Cys replacements introduced into the protein. With this approach we succeeded to show that Asp133 which is located at the unique structural fold changes conformation with pH [30]. d) The global structural dynamics of NhaA. Using two computational approaches we modeled the outward facing conformation of NhaA and its possible alternative conformational change [31] Recently, the Padan's and Michel's groups adopted a MASS spectrometry technique (HDX, hydrogen/deuterium exchange) to follow experimentally the global structural dynamics of NhaA [32]. Two sets of ligand-induced concerted movements of helices have been revealed which were not seen before. These movements initiate the activation of NhaA. e) NhaA-based models of two humen antiporters. Based on the crystal structure of NhaA we have modeled NHE1 [33], a house keeping Na^+/H^+ antiporter that plays a primary role in certain cardiac conditions; and NHA2 [34], an NhaA orthologue suggested to be an essential factor in essential hypertension. These will form the first steps toward rational drug design.

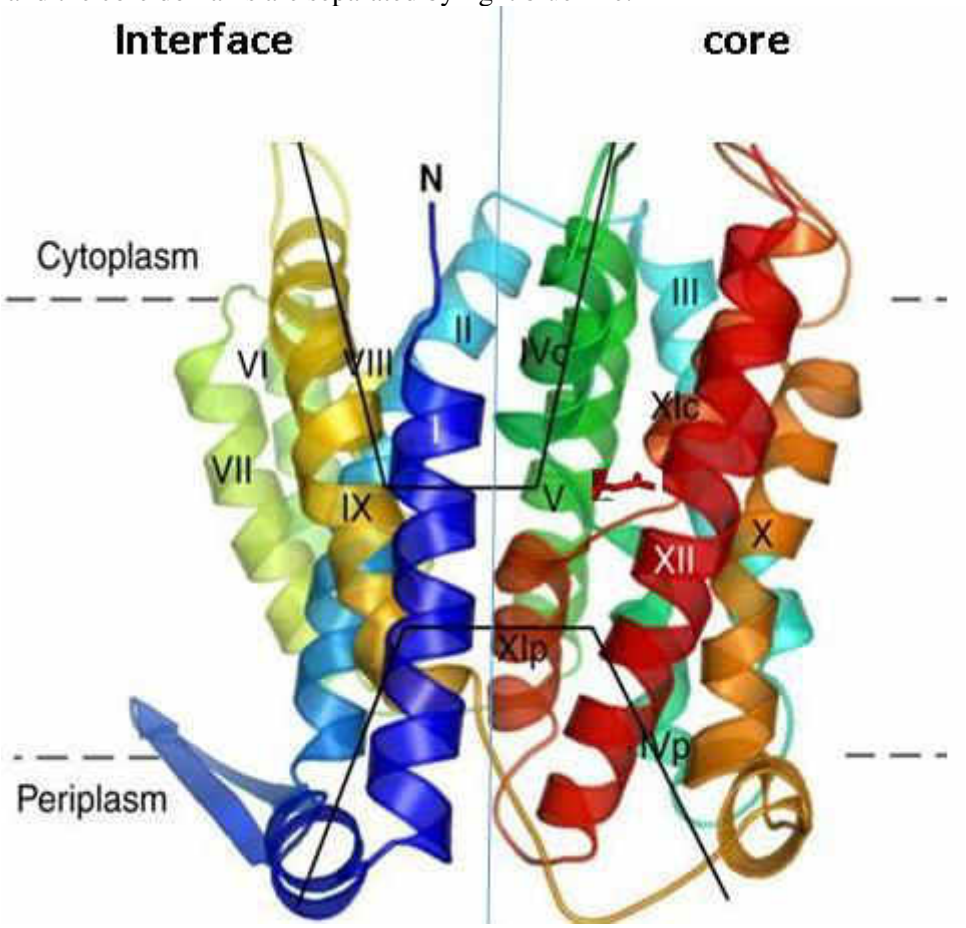
References

1. Krulwich, T. A., Sachs, G. & Padan, E. (2011). Molecular aspects of bacterial pH sensing and homeostasis. *Nat Rev Microbiol* **9**, 330-43.
2. Padan, E. (2014). Functional and structural dynamics of NhaA, a prototype for Na(+) and H(+) antiporters, which are responsible for Na(+) and H(+) homeostasis in cells. *Biochim Biophys Acta* **1837**, 1047-62.
3. Orlowski, J. & Grinstein, S. (2007). Emerging roles of alkali cation/proton exchangers in organellar homeostasis. *Curr Opin Cell Biol* **19**, 483-92.
4. Fliegel, L. (2008). Molecular biology of the myocardial Na+/H+ exchanger. *J Mol Cell Cardiol* **44**, 228-37.
5. Padan, E. & Landau, M. (2016). *Sodium-proton (Na^+/H^+) antiporters: properties and roles in health and disease in The alkali metal ions: their role for life*. Metal ions in life sciences (Sigel, A., Sigel, H. & Sigel, R. K. O., Eds.), 16, Springer International, Cham, Switzerland.
6. Padan, E., Bibi, E., Ito, M. & Krulwich, T. A. (2005). Alkaline pH homeostasis in bacteria: new insights. *Biochim Biophys Acta* **1717**, 67-88.
7. Padan, E., Venturi, M., Gerchman, Y. & Dover, N. (2001). Na(+)/H(+) antiporters. *Biochim Biophys Acta* **1505**, 144-57.
8. Brett, C. L., Donowitz, M. & Rao, R. (2005). Evolutionary origins of eukaryotic sodium/proton exchangers. *Am J Physiol Cell Physiol* **288**, C223-39.
9. Taglicht, D., Padan, E. & Schuldiner, S. (1991). Overproduction and purification of a functional Na+/H+ antiporter coded by nhaA (ant) from Escherichia coli. *J Biol Chem* **266**, 11289-94.
10. Dwivedi, M., Sukenik, S., Friedler, A. & Padan, E. (2016). The Ec-NhaA antiporter switches from antagonistic to synergistic antiport upon a single point mutation. *Sci Rep* **6**, 23339.
11. Orlowski, J. & Grinstein, S. (2004). Diversity of the mammalian sodium/proton exchanger SLC9 gene family. *Pflugers Arch* **447**, 549-65.
12. Putney, L. K., Denker, S. P. & Barber, D. L. (2002). The changing face of the Na+/H+ exchanger, NHE1: structure, regulation, and cellular actions. *Annu Rev Pharmacol Toxicol* **42**, 527-52.
13. Wakabayashi, S., Hisamitsu, T., Pang, T. & Shigekawa, M. (2003). Kinetic dissection of two distinct proton binding sites in Na+/H+ exchangers by measurement of reverse mode reaction. *J Biol Chem* **278**, 43580-5.
14. Padan, E. (2008). The enlightening encounter between structure and function in the NhaA Na+-H+ antiporter. *Trends Biochem Sci* **33**, 435-43.
15. Hunte, C., Screpanti, E., Venturi, M., Rimon, A., Padan, E. & Michel, H. (2005). Structure of a Na+/H+ antiporter and insights into mechanism of action and regulation by pH. *Nature* **435**, 1197-202.
16. Lee, C., Yashiro, S., Dotson, D. L., Uzdavinys, P., Iwata, S., Sansom, M. S., von Ballmoos, C., Beckstein, O., Drew, D. & Cameron, A. D. (2014). Crystal structure of the sodium-proton antiporter NhaA dimer and new mechanistic insights. *J Gen Physiol* **144**, 529-44.
17. Padan, E., Venturi, M., Michel, H. & Hunte, C. (1998). Production and characterization of monoclonal antibodies directed against native epitopes of NhaA, the Na+/H+ antiporter of Escherichia coli. *FEBS Lett* **441**, 53-8.
18. Padan, E. & Michel, H. (2015). NhaA, a unique structural fold of secondary active transporters. *Israel J. Chem.* **55**, 1233-1239.
19. Lee, C., Kang, H. J., von Ballmoos, C., Newstead, S., Uzdavinys, P., Dotson, D. L., Iwata, S., Beckstein, O., Cameron, A. D. & Drew, D. (2013). A two-domain elevator mechanism for sodium/proton antiport. *Nature* **501**, 573-7.
20. Shi, Y. (2013). Common folds and transport mechanisms of secondary active transporters. *Annu Rev Biophys* **42**, 51-72.
21. Paulino, C. & Kuhlbrandt, W. (2014). pH- and sodium-induced changes in a sodium/proton antiporter. *Elife* **3**, e01412.
22. Wohlert, D., Kuhlbrandt, W. & Yildiz, O. (2014). Structure and substrate ion binding in the sodium/proton antiporter PaNhaP. *Elife* **3**, e03579.
23. Jardetzky, O. (1966). Simple allosteric model for membrane pumps. *Nature* **211**, 969-70.
24. Kaback, H. R. (2015). A chemiosmotic mechanism of symport. *Proc Natl Acad Sci U S A* **112**, 1259-64.
25. Ganea, C. & Fendler, K. (2009). Bacterial transporters: charge translocation and mechanism. *Biochim Biophys Acta* **1787**, 706-13.
26. Zuber, D., Krause, R., Venturi, M., Padan, E., Bamberg, E. & Fendler, K. (2005). Kinetics of charge translocation in the passive downhill uptake mode of the Na+/H+ antiporter NhaA of Escherichia coli. *Biochim Biophys Acta* **1709**, 240-50.

27. Mager, T., Rimon, A., Padan, E. & Fendler, K. (2011). Transport mechanism and pH regulation of the Na+/H+ antiporter NhaA from Escherichia coli: an electrophysiological study. *J Biol Chem* **286**, 23570-81.
28. Calinescu, O., Dwivedi, M., Patino-Ruiz, M., Padan, E., and Fendler, K. (2017). Lysine300 is essential for stability but not for electrogenic transport of the E. coli NhaA N^+/H^+ antiporter. *J. Biol. Chem.* **292**, 7932-41
29. Kozachkov, L. & Padan, E. (2011). Site-directed tryptophan fluorescence reveals two essential conformational changes in the Na+/H+ antiporter NhaA. *Proc Natl Acad Sci U S A* **108**, 15769-74.
30. Rimon, A., Kozachkov-Magrisso, L. & Padan, E. (2012). The unwound portion dividing helix IV of NhaA undergoes a conformational change at physiological pH and lines the cation passage. *Biochemistry* **51**, 9560-9.
31. Schushan, M., Rimon, A., Haliloglu, T., Forrest, L. R., Padan, E. & Ben-Tal, N. (2012). A model-structure of a periplasm-facing state of the NhaA antiporter suggests the molecular underpinnings of pH-induced conformational changes. *J Biol Chem* **287**, 18249-61.
32. Eisinger, M. L., Dorrnaum, A. R., Michel, H., Padan, E., and Langer, J. D. (2017). Ligand-induced conformational dynamics of the *Escherichia coli* Na^+/H^+ antiporter NhaA revealed by hydrogen/deuterium exchange mass spectrometry. *Proc Natl Acad Sci U S A* **114**, 11691-11696
33. Landau, M., Herz, K., Padan, E. & Ben-Tal, N. (2007). Model structure of the Na+/H+ exchanger 1 (NHE1): functional and clinical implications. *J Biol Chem* **282**, 37854-63.
34. Schushan, M., Xiang, M., Bogomiakov, P., Padan, E., Rao, R. & Ben-Tal, N. (2010). Model-guided mutagenesis drives functional studies of human NHA2, implicated in hypertension. *J Mol Biol* **396**, 1181-96.

Figure 1. The architecture of NhaA

A ribbon presentation of the crystal structure of NhaA viewed parallel to the membrane (broken line) The 12 trans membrane segments (TM) are labelled with Roman numerals. N and C indicate the N and C termini. The cytoplasmic and periplasmic funnels are marked by black lines. The interface and the core domains are separated by light blue line.



Robotics and New Energy System Research

by Aarne Halme, Member EUAS

Short Biography

Aarne Halme is emeritus professor of Aalto University (before Helsinki University of Technology), Finland, and Chairman of the Board of GIM Ltd. His background is in control and systems engineering. He started academic carrier in 1972 as an associate professor of control engineering at Tampere University of Technology. In 1977 he moved to Oulu University, where he was professor of control and systems engineering. From 1986 until retirement he has been professor of automation technology at Helsinki University of Technology, where the period 2008-2013 he was the head of the Academy of Finland Centre of Excellence in Generic Intelligent Machines. After retirement 2014 he established with his colleagues GIM Ltd (www.gimltd.fi) which continues the activities of the Excellence Centre on commercial bases. He has made both theoretical and practical research in many fields of systems science and automation. Since mid 80's he has worked actively with intelligent field and service robotics research including development of mobility means, like walking and hybrid mechanisms, navigation and perception systems, and interactive human robot interfaces. His scientific interest includes also new energy technologies especially fuel cell systems intended to use in mobile devices. Publishing includes more than 200 articles in scientific journals and conferences.

Robotics

My current research in robotics is concentrated on field and service robotics which are robotic machines that work outside factories replacing people in tasks, which are monotonous or which do not any more fulfill the minimum requirements for human work. They operate often in an environment unfriendly for humans or offer help or entertainment services to people in their homes and public places. Task scenario usually includes an environment, which is not well structured, not a priori known in details and may be changing with time. Often high autonomy is needed. Such environments are typical also for biological species. In most cases robots must be mobile, because tasks cannot be moved to the robots (like in factories), but robots must move to the tasks. Research and development of field and service robots has been very active since mid 80s and we have seen many interesting robots in media.. It is important to note that appearance of those robots may vary a lot depending on their application field, size and tasks they are intended. Human like robots are rather exceptions than the rule. Many field robots are designed by automating existing work machines. In the figure below some of those robots are visualized.

In field robotics application vary from farming, construction and utilization of natural resources like mining, to exploration of planetary system (moon, planets, asteroids). Important application field is also undersea operations, where robots replace people in deep waters. In service robotics home services, entertainment, disabled support, replacing manpower in human-intensive non-industrial work in offices, hospitals, public places, hostile urban environment (cleaning streets, sewers etc) are the main application areas. Outside normal civil tasks military technology, rescue operations and catastrophe aftercare also use robots today.

Challenges in Modern Robotics

There are two challenging technological steps for robots in their way from factories to among people. The first to be taken is to obtain fluent mobility in unstructured, changing environments, and the second is to obtain the capability for intelligent communication with humans together with a fast, effective learning/adaptation to new work tasks. The first step has almost been taken today. The rapid development of sensor technology – especially inertial sensors and laser scanners – with constantly increasing processing power, which allows heavy image processing and techniques for simultaneous localization and mapping (SLAM), have made it possible to allow slowly moving robots to enter in the same areas with humans. However, if we compare the present capability of robots to animals, like our pets in homes, it can be said without no doubt that improvements are still possible and desirable.

The second step is still far away. Traditional industrial robots are mechanically capable to change a tool and perform different work tasks, but due to the nature of factory work need for reprogramming is relatively minor and therefore interactive communication with the user and continuous learning are not needed. The most sophisticated programming methods allow task design, testing, and programming off-line in a simulation tool without any contact to the robot itself. Today's commercial mobile service robots, like vacuum cleaners and lawn mowers, are limited to a single task by their mechanical construction. A multi-task service robot needs both mechanical flexibility and a high level of "intelligence" in order to carry out and learn several different tasks in continuous interaction with the user. Instead of being a "multi-tool" the robot should be capable of using different kinds of tools designed for humans. Due to fast development in mechatronics, hardware is not any more the main problem although the prices can be high. The bottlenecks are the human – robot interface (HRI) and the robot intelligence, which are strongly limiting both the information transfer from the user to the robot as well as the learning of new tasks.

Despite huge efforts in AI and robotics research, the word "intelligence" has to be written today in quotes. Researchers have not been able to either model or imitate the complex functions of human brains or the human communication, thus today's robots hardly have either the creativity or the capacity to think. The main requirement for a

service robot HRI is to provide easy humanlike interaction, which on the one hand does not load the user too much and on the other hand is effective in the sense that the robot can be kept in useful work as much as possible. Note that learning of service robots new tasks is not counted as useful work! The interface should be natural for human cognition and based on speech and gestures in communication. Because the robot cognition and learning capabilities are still very limited the interface should be optimized between these limits by dividing the cognitive tasks between the human brains and robot "intelligence" in an appropriate way. The answer is to use multi-modalities i.e use all communication means natural to human to communicate the task to the robot. This means using audio-visual means together with traditional IT-communication means. The picture below illustrates a robot, called WorkPartner, and a task (cleaning snow from yard) we have used to research different means to communicate the task effectively on-line to the robot. In this case we utilize human cognition and common spatial awareness of the robot and the human. The key component in communication is a sign showing position and direction which the robot can read by camera vision. The software recognize the task details and control the robot after the human has marked off the area to be cleaned and gives voice commands define the details of the work (like where to heap the snow). By this way we avoid the time consuming use of map based configuring of the task which is be the traditional way doing it.

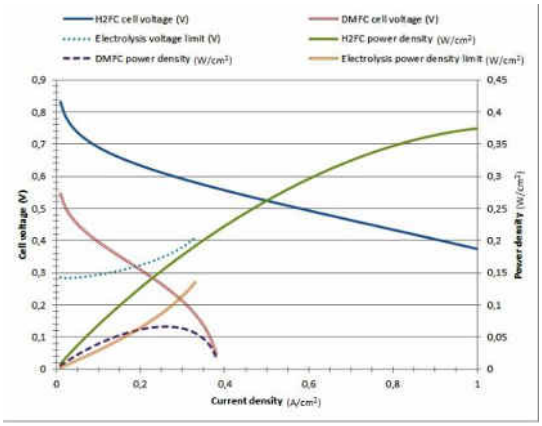
More details on this topic and the story of WorkPartner robot, which is one of the world's most advanced service robot, can be found from articles listed references.

New Energy Technology – Nonconventional Fuel Cells

Availability of energy is a basic issue in all mobile devices. My research in this field concerns new fuel cell technology that utilize biological catalysts or platinum catalyst in unconventional way. We have done this research since beginning of 90'. The latest results concern alternative concept for Direct Methanol Fuel Cell (DMFC) showing that in certain conditions combination of an electrolyser reforming methanol and a PEM fuel cell is more efficient than DMFC having also some other advantages. This is due to the very low energy, in practice only 0,7-1.0 W/LH2, needed to reform aqueous methanol by electrolysis in low temperature (20-50 Celsius). This corresponds 0, 3-0,4 V cell voltage in an electrolyser cell (depending on the operating point). At such voltages water is not split. Taking into account that HHV of hydrogen is 3,5 W/LH2 and a PEM fuel cell produces electricity about 50% efficiency there is still energy left for application use even if the electrolyser power is taken from a PEM fuel cell where the hydrogen is fed. The interconnected system can thus act like a conventional DMFC producing autonomously electrical energy from aqueous methanol. The figure below compares the new concept to

DMFC and demonstrates some of its advantages, like a better efficiency in certain conditions and ability to operate in much higher methanol concentrations without catalyst poisoning risk. In my knowledge this is the first time when the concept has been introduced in the scientific literature (more details can be found in the article in the reference list).

Before the above research my research was more than 20 years with biological fuel cells, first using bacteria as catalyst and later using MDH enzyme as catalyst and aqueous methanol as fuel. In both cases we have succeeded to make well working fuel cells being pioneers in the field. Bacteria fuel cells can utilize very large variety of fuels (subrates), for example different biodegradable wastes, stabilizing them at the same time when taking out electrical energy. An interesting example is a study we made for ESA how to use this technology as part of energy recovery system in future manned flights to Mars. In the long flights all human food residuals and secrets are circulated and energy included is recovered. Enzyme catalysed fuel cells were researched and developed a small scale power source in mind for portable electronic devices. We ended up to methanol because of its excellent ability to carry hydrogen energy. Direct methanol biofuel cell was the first one of its kind when published. It was also patented. Using MDH enzyme as the catalyst is the key issue in it, because being so called PQQ dehydrogenase, which need not NADH cofactor to operate, it is more stable and easy to use in applications than some other enzymes



References

Halme A., Leppänen I., Suomela J., Ylönen S., Kettunen I., WorkPartner: Interactive human-like service robot for outdoor applications, International Journal of Robotics Research ,22, 7-8 SPECIAL ISSUE, 2003

Halme A., Common Situation Awareness as Basis for Human-Robot Interface, Climbing and Walking Robots pp 3-18, Springer,2006

Heikkilä M., Terho S., Hirsi M., Halme A., Forsman P., Using signs for configuring work tasks of service robots, Industrial Robot ,33, 4, 2006

Halme A., Luksch T., Ylönen S. Biomimicing motion control of the WorkPartner robot, Industrial Robot , 31,2, 2004

Ylönen S.J., Halme A.J.,WorkPartner - Centaur like service robot, IEEE International Conference on Intelligent Robots and Systems , 2002

Suomela J., Halme A., Novel interactive control interface for centaur-like service robot, IFAC Proceedings Volumes (IFAC-PapersOnline), 15,1, 2002

Heikkilä, S., Halme A., Affordance-Based Indirect Task Communication for Astronaut-Robot Cooperation, Schiele, A., Journal of Field Robotics 29(4), 2011

Halme, A., Selkäinaho, J., Noponen, T., & Kohonen, A., An alternative concept for DMFC - combined electrolyzer and H2 PEMFC. International Journal of Hydrogen Energy, 41(4),2016

Zhang X.-C., Ranta A., Halme A., Direct methanol biocatalytic fuel cell-Considerations of restraints on electron transfer", Biosensors and Bioelectronics, 21, 11, 2006

Zhang X.-C., Halme A., Modelling of a microbial fuel cell process, Biotechnology Letters, 17 ,8, 1995

Halme, A Biomass Based Fuel Cells - Application to Manned Space Exploration, ACT Workshop on Innovative Concepts . ESA-ESTEC 28-29 January 2008.

Innovative Methods in Airway Disease Research

by Peter Barnes, Member EUAS

Short Biography

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

Education:

1966-69 Preclinical: Cambridge University (St Catharine's College)(Double first degree)
Open Scholarship, elected to title of Scholar
1969-72 Clinical: Oxford University Medical School (Clinical Scholarship)

Previous appointments:

1975-1978: Registrar (General Medical Rotation), University College Hospital, London
1978-1979: MRC Research Fellow and Honorary Senior Registrar, Dept of Clinical Pharmacology, Royal Postgraduate Medical School, London
1979-1982 Senior Registrar (Resp Medicine) Hammersmith Hospital, London
1981-1982 MRC Travelling Fellowship to CVRI, University of California
1982-1985 Consultant Physician, Hammersmith Hospital, London
1985-1987 Professor of Clinical Pharmacology, Cardiothoracic Institute

Current Appointment (since 1987): funded by HEFCE

Margaret-Turner-Warwick Professor of Thoracic Medicine, National Heart & Lung Institute
Head of Respiratory Medicine, Imperial College
Honorary Consultant Physician, Royal Brompton Hospital

Degrees, Honours and Awards

1982 DM: Oxford University (Thesis: Adrenergic mechanisms in asthma)
1986 FRCP: Royal College of Physicians
1987 DSc: Oxford University
1990 Linacre Lecture, Royal College of Physicians, London
1994 Goldberg Prize, University of Chicago
1996 Amberson Lecture, American Thoracic Society (most prestigious lecture)
1997 Honorary MD, University of Ferrara, Italy
1998 Fellow Academy of Medical Sciences (FMed Sci, Founding Fellow)
1999 Sadoul Lecture, European Respiratory Society (most prestigious lecture)
2000 Honorary MD, University of Athens, Greece
2005 Honorary MD, University of Tampere, Finland
2007 Fellow of Royal Society (first respiratory scientist for >150 years)
2007 Presidential Award, European Respiratory Society
2008 British Thoracic Society Gold Medal
2009 NIHR Senior Investigator
2009 Croonian Lecture, Royal College of Physicians, London
2010 Honorary MD, Leuven University, Belgium
2011 Honorary Fellow of St Catharine's College, Cambridge
2012 Member of Academia Europaea (Academy of Europe, MAE
Master Fellow, American College of Chest Physicians (one of only 2 outside N America)
2013-2014 President of European Respiratory Society (largest respiratory society in the world)
2014 Honorary degree, Maastricht University, Holland
Elected Member of Association of American Physicians
Wellcome Lecture, Royal Society of Medicine (most prestigious lecture)
2015 Galen Medal, Society of Apothecaries, London (most prestigious award)
President's Award for Scientific Innovation, Imperial College

Research

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

Recent research funding

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

University Spin-out Company

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

Editorial

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

Publications

Over 1000 peer reviewed publications. Most highly cited respiratory researcher in the world and most highly cited clinical researcher in Europe over last 25 years (h-index = 156, >120,000 citations)
17th most highly cited scientist ever in the world. Author and editor of over 50 books on airway disease and pharmacology.

Research summary

Peter Barnes is one of the leading respiratory scientists in the world and is known for his research into mechanisms and treatment of asthma and chronic obstructive pulmonary disease (COPD), two of the most prevalent disease in the world today. He has been the most highly cited respiratory researchers in the world over the last 30 years, as well as the most highly cited clinical scientist in Europe, and amongst the top 20 scientific citations in the world, with a current h-index of 160 (Web of Science).

He has been a prolific and imaginative researcher in exploring many areas of science related to asthma and COPD, taking a broad multidisciplinary approach from molecular and cell biology through to clinical studies. He has been at the forefront of translational research in respiratory medicine for four decades.

Peter Barnes has explored the nature of inflammation in asthma, the role of different inflammatory mediators in this disease and how they contribute to airway hyperresponsiveness and symptoms. His initial research focussed on neural and autonomic mechanisms of airway control, the role of adrenergic mechanisms and the contributions of various neuropeptides that are localised to nerves in human airways. He was the first to

map out adrenergic and cholinergic receptors in the lungs and to describe their function and regulation. Many of the treatments used for asthma and COPD work by interacting with these autonomic receptors, thereby providing new insights into the mechanism of actions of beta-adrenergic agonists and anticholinergics (muscarinic receptor antagonists), which are the main bronchodilator classes used today.

He discovered the long duration of action of the muscarinic antagonist tiotropium bromide, showing how it was effective with once daily dosing. This has now become the greatest selling bronchodilator for use by COPD patients. He also discovered that another related drug, glycopyrrolate, previously used in other indications, had prolonged effects on airway muscarinic receptors and has subsequently been developed for clinical use as an inhaled drug for COPD.

Professor Barnes identified non-adrenergic bronchodilator nerves in human airways and showed that the neurotransmitter of these nerves was nitric oxide (NO) and that this mechanism is defective in asthma, contributing to airway hyperresponsiveness in this disease.

His extensive research to uncovered the molecular basis for the anti-inflammatory effects of corticosteroids in asthma demonstrating the importance of histone acetylation in activating multiple inflammatory genes in asthmatic airways and the role of corticosteroids in recruiting histone deacetylase-2 (HDAC2) to reverse this acetylation and switch off inflammatory genes. In contrast to asthma, COPD is resistant to the anti-inflammatory effects of corticosteroids shown to be the consequence of a marked reduction in HDAC2 activity by the high oxidative stress in COPD. This effect of oxidative stress was mediated through the activation of phosphoinositide-3-kinase, so that PI3K inhibitors were able to reverse corticosteroid resistance in COPD cells. This effect was mimicked by the long used anti-asthma drug, theophylline, but at lower concentrations than normally used. This has led to clinical trials of low dose theophylline in COPD and severe asthma and the establishment of an Imperial College spin-out company called RespiVert which developed highly potent inhaled inhibitors of this pathway. After acquisition by Janssen Pharmaceuticals these drugs are now in clinical development.

Another area that he has pioneered is the measurement of biomarkers of inflammation in the breath to diagnose airway disease and monitor the effects of therapy. His lab was the first to show how exhaled NO can be used to monitor the effects of inhaled corticosteroids in asthma. The technique of exhaled NO has now become a standard tool for monitoring asthma in clinical practice. He has explored other biomarkers in exhaled breath condensate including various inflammatory mediators that are also abnormal in patients with asthma and COPD.

More recently, his research has focussed on the basic mechanisms underlying COPD. A characteristic of COPD patients is that their lower airways and lungs are colonised with certain bacteria such as *Haemophilus influenzae*. He went on to show that this persistence of microorganisms was explained by defective removal of bacteria by alveolar macrophages on account of dysregulation of microtubules in these cells.

Another important area of research is into mechanism of accelerated ageing in the lung which is found in COPD and lung fibrosis. There is an accumulation of senescent cells in the lungs due to loss of anti-ageing molecules such as sirtuins which are reduced by oxidative stress through the activity of particular micro-RNAs. By blocking the critical micro-RNAs, it is possible to reverse senescence in COPD cells with potential novel therapeutic applications. His current research is exploring the molecular pathways leading to cellular senescence in COPD and how existing therapies may be repurposed and novel therapies developed to prevent the development of senescence in COPD and its comorbidities.

Publications

Over 1,100 papers in peer-reviewed journals, with >110,000 citations and average citations 56.5/article.

He has also edited, written or co-edited over 50 books on asthma, COPD and respiratory pharmacology.

Full publication list: https://scholar.google.com/citations?user=z5PuQ_0AAAAJ&hl

Biomimetic Physics: Learning from Evolutionary Strategies of Overcoming Evolutionary Crises. Nature as Material Designer

by Erich Sackmann

Short Biography

Biographical Sketch:

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

1974 he became Full Professor of Physics and head of the biophysics department at the University of Ulm. From1980 to 2003 he held the chair of Biological Physics at the Physics Department of the Technical University Munich. He presently works as Professor Emeritus at the Technical University Munich and the Ludwig Maximilian University Munich.

Professional Activities:

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

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

Awards

2001 Oswald Award, German Colloid Society
Fellow of the American Physical Society 2002
2004 Regents professorship of University of California (UCLA)
2006 Stern-Gerlach Medal of the Deutsche Physikalische Gesellschaft

Abstract

The evolution of the sheer infinite manifold of living beings has been realized with an astonishing small number of organic molecules. This was achieved by interplay of physics chemistry and genetics and the concept of hierarchical design. Many concepts of human rational design of smart materials have been invented by Mother Nature several billion years ago. Nature can teach us how to design highly sophisticated mechanical structures and systems comprising length scales from nanometer to meters by hierarchical design from functional modules (such as lipid membranes, ion pumps or rotating and linear molecular motors). Here I attempt to show that we can learn much on the design of smart materials and robots by studying the behavior of animals surviving under harsh condition, such as living in the desert. As an example I consider here the swimming of sandfish below sand.

Introduction

The development of new biological concepts or devices took place in quantum jumps which were driven by life threatening evolutionary crises. Intensive studies of these questions are expected to lead to new strategies for solving major future challenges, including global chronic food shortage, global heating and even social conflicts. Of course we can never verify models or scenarios of biological evolution by experiments. However, the occupation with these fascinating questions stimulates the interdisciplinary cooperation and the education of a new generation of students who are better suited to solve future ecological crises then the present societies.
Three outstanding examples are:

- First, the evolution of photosynthetic devices enabling the storage of energy be electrochemical gradients across bio-membranes which drive the generation of ATP and, most importantly, nature's introduction of the nanoscopic water splitting manganese protein assemblies (see reference [1]).
- Second, the design of new materials with unique physical properties enabling animals (such as sand fish) to survive under extreme environmental conditions (such as the deserts).
- The rapid switching of rotating direction of bacterial motors by (Martensitic like) solid-solid phase transitions. I

The first example was considered in detail in [1] whereas in this contribution I concentrate on the second issue. The third example is described in the Erich Sackmann: Lecture Notes in biological Physics: Lecture "Bionics" accessible via www.biophy.de

Swimming in the Sahara Sand

Physicists or engineers who are involved in the design of new materials can learn much by studying living matter. Mother Nature developed a manifold of smart materials to optimize motional processes or to protect animals from external hazards. One stunning example is the sandfish of genus *Scincus*, a lizard which can dive deep into the desert sand and move with velocities of 0.1 m/sec (or 0.36 km/h), hence the name sandfish (see Figure 1 and [2]). Below sand, the animals move by exciting bending waves traveling from head to tail, while the feet most likely serve mainly the motion on the surface. This method of self-propulsion is remarkably similar to that of bacteria swimming in water or to snails crawling in grass as we will see below.

The motion of sandfish below desert sand is determined by two physical scaling concepts: the swimming of small objects at very high friction (or high Reynolds numbers) and the reduction of solid friction by specific design of its skin. The sandfish skin is an impressive example of the evolution of smart surfaces that control the contact of living systems with the environment. Other examples of nature as surface designer (not considered here) are the control of wetting of leafs by water, mediated by adjusting the surfaces roughness, (often called Lotus-effect) and the generation of shells with outstanding mechanical properties by bio-mineralization (reviewed by [3]).

Self-propelled swimming of long objects at very low Reynolds numbers

There are close analogies between the swimming of bacteria and sandfish although the properties of water and granular media are very different. To show this analogy we first address the question: why bacteria cannot swim like fish or humans in water by moving their appendages? The reason is that nature had to account for the scaling laws of physics. Fish swim by generating hydrodynamic flow fields moving towards their back side. The well-known laws of hydrodynamics of viscous fluids teach us that the flow velocity is zero at the surface resulting in a velocity gradient $\partial v / \partial z$ perpendicular to the surface (defined as z-axis) which generate a Newton frictional force

$$F_f = \eta \frac{dv}{dz} \tag{1}$$

where η is the viscosity of the fluid. To fulfill the condition of force equilibrium at the surface (Newton's third law) the frictional tension generates the momentum for the advancement of the body. In inhomogeneous flow fields the molecules are also subjected to inertial forces f_i (per unit volume) since they change their velocity vector while moving in the direction of the gradient:

$F_i = \rho \vec{v}\, grad\, \vec{v}$, where ρ is the mass density. Taken together these consideration show that swimming is determined by the interplay of frictional and inertia forces. The swimming behavior of animals is therefore determined by the dimensionless Reynolds number Re which is equal to the ratio of the accelerating force to the frictional force:

$$\mathrm{Re} = \frac{\rho v^2 L^2}{\eta L v} \qquad (2)$$

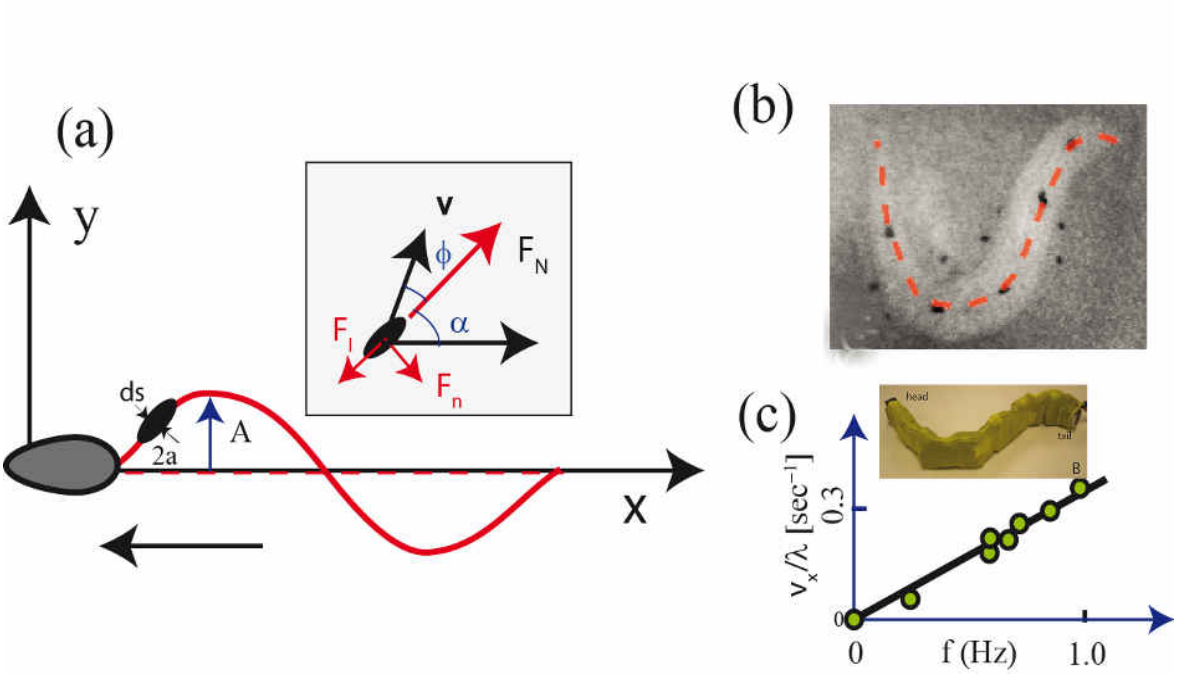


Figure 1: *(a) Definition of forces on local segments of flagella or snake like animals (water snake or sperm cells) moving by agitating of travelling waves of amplitude A and angular frequency along the elongated body from head to tail. v is the local velocity of the segment, F_p and F_n are the forces parallel and perpendicular to the local segment and (b) snapshot of sand fish moving below sand visualized by X-ray imaging (modified according to [4]). (c) Measurement of normalized velocity of model sandfish (see inset) as function of frequency of excitation (redrawn according to [4])*

Dimensionless numbers such as Re play key role for the design of ships and airplanes since they shows the engineer how the behavior of his design depends on the size L and the density ρ of the medium. In particular, he knows that a large ship swimming in water behaves as a small model swimming in mercury. It was first recognized by Galilei that natural evolution was guided by scaling laws. An impressive example is the change of the swimming behavior of fish and bacteria. For a typical fish (L~ 1m, v ~ 10m/sec) Re ~10^4 and the energy dissipated is very small. For a cylindrical fish of circumference B the force is of the order $F_r = -\eta \frac{dv}{dz} B\, L$. For bacteria (L~1µm, v~10µm/sec) the Reynolds number is of the order of Re~10^{-6}. Therefore nearly all energy generated by the motor is dissipated into heat. In summary, bacteria moving in water feel like a fish swimming in honey [5].

There was another problem nature had to solve during evolution by using flagella as agitator of motion. Long cylinders behave very different from spheres. The laminar flow field decays very slowly with distance: $v \propto r^{-1}$ and a moving cylinder has to carry much more fluid than a sphere (see [6] § 20). Fortunately these problems are less severe for rapidly oscillating long objects as was first recognized by the most prominent 21th century expert in hydrodynamics G. Tayor [5]. In a celebrated paper he showed that small animals with flagella can swim if they generate traveling undulation waves running from the head to the tail (such as rope waves), thus generating a force directed opposite to the direction of the wave. For cylindrical objects of radius a the velocity is related to the phase velocity U of the wave given by :

$$v = \frac{1}{2} A^2 q^2 \frac{K_0(qa) - 1/2)}{K_0(qa) + 1/2} U \quad (3)$$

where q is the wave vector $q = \frac{2\pi}{\lambda} = \frac{2\pi\nu}{U}$, K_0 is the Bessel function of first kind and U the phase velocity. Please note that this equation holds not only for unicellular organisms (such as sperm) or rod shaped animals (such as snails) which excite planar oscillations but also for the E. coli bacteria rotating their helical shaped flagella, since the rotating wave can be decomposed into two perpendicularly oriented planar waves phase shifted by $\pi/2$. The most important result is that the velocity is a quadratic function of the undulation amplitude and the frequency. Thus the self-propelling of bacteria is an effect of second order. Taylor designed macroscopic artificial animals with rotating motors to verify his theory. He showed in these experiments that the swimming technique of bacteria works only at high Reynolds numbers.

The analogy between the swimming of sandfish and bacteria becomes evident if we have a closer look at the physical basis of the propulsive force (see Figure 1). We consider the frictional force on a flagella segment of length δl moving with momentary velocity v. The frictional force on the element is $\delta \mathrm{F} = \zeta_{\mathrm{n}} v_n + \zeta_{\mathrm{p}} v_p$ where v_n and v_p are the velocities and ζ_p and ζ_{p} the frictional coefficients in the tangential and normal direction [8]. The key point is the anisotropy of the frictional forces. In liquids, the frictional force in the tangential direction is $\zeta_{\mathrm{n}} \approx 2\pi\eta L / k_B T \ln L/a)$ and is by a factor of 2 smaller than in the normal direction: ζ_p / ζ_n =1/2. A closer inspection of Figure 1 shows that the resulting frictional force on an element δl moving with an oblique angle ϑ with respect to the body axis is:

$$F_{res} \approx \zeta_p v_p \cos\vartheta . \quad (4)$$

According to Newton's third law F_{res} is a measure for the propulsion force. It is determined by the anisotropic friction exerted by the moving fluid on the flagella. As pointed out already by Taylor, the bacteria and sperm swim in fluids as screws that are driven into the wall by rotating with a screw driver.

Let us now consider the situation for sandfish. Similar to flagella of sperm or snakes, it generates propulsion forces by agitating travelling bending waves moving along its slender body. As in the case of bacteria the driving force is determined by the direct frictional coupling of the sand particles with the skin. The major difference is that the sand is a viscoelastic medium and the motion is also controlled by the deformation of the sand by the moving animal [4]. Following a theory by Herrmann et al [9] the forces on a small surface element of the body moving in sand can be expressed as:

$$F_n = k\delta^{3/2} - G'' v_N \delta^{1/2} \quad (5a) \qquad \text{and} \qquad F_{fp} = \mu F_n \quad (5b)$$

The right term of Equation (5a) accounts for the elastic deformation of sand and is expressed in terms of the Hertz model of deformation of elastic bodies by a small objects. Therefore, k is an effective elastic constant and μ the indentation induced by the normal force. The right term accounts for the energy dissipation by friction, where G'' is the effective loss modulus of the sand and v_n is the normal velocity. Equation (5b) is the classical Coulomb equation of the effective frictional force in the tangential direction.

Similar to Taylor a group of engineers at the Georgia Tech designed robots which can mimic the motion of sandfish (see [4]). The robots are composed of arrays of small cylinders which can rotate about an axis perpendicular to the plane of undulation. By periodically rotating (see Figure 1c) the segments by small angles the robots can mimic the locomotion of snakes. In a separate experimental study by Ding et al. it was shown that one can calculate the frictional force on a long cylinder moving in sand by dividing its surface into small plates and integrate over the forces on all of these elements. The pertinent results of these studies are [10]:

- The locomotion of snakes or sandfish on the surface or within sand is determined by the anisotropic frictional force on the surface, in analogy to the swimming in fluids at very small Reynolds numbers.

- The swimming velocity is a linear function of the undulation frequency. This contrasts ith the swimming of slender objects in water where the velocity depends on the square of the amplitude and frequency.
- The mechanism of force generation in sand is different from that applied by worm like animals (snakes, lizards or nematodes) to move on granular surfaces. In the latter case forward thrust is generated by the resistive forces arising by pushing the body sideward.

The role of the feet of sandfishes is still debated. The X-ray studies suggest that the feet lie close to the body and play a minor role. An argument in favour of this conclusion is the good agreement between the calculated and the observed motions of the sandfish robot [4]. On the other side Baumgartner and coworkers provided evidence that the feet perform "paddling-like movements" and in this way enforce the thrust [7].

Design and tribology of sandfish and snake skin.

We consider now the question how the animals skin can resist the abrasive force generated by the strong friction.

The outer skin of reptiles (called Oberhäutchen) is covered by a thin layer of β-keratin forming beta pleated sheets such as silk. On the surface of snakes the β -keratin forms about 5 µm long and 100-nm thick hairs (microfibrils) which lie flat on the surface and point all with the ends towards the rear end (see Figure 2, right side).The loose end points slightly upwards acting as barbs that render the friction lower when the snakes move forward but higher if they move backwards or laterally. A very remarkable feature in the case of snakes is the small pores with 30-50 nm diameter which may serve the secretion of lubricant or the uptake of moisture.

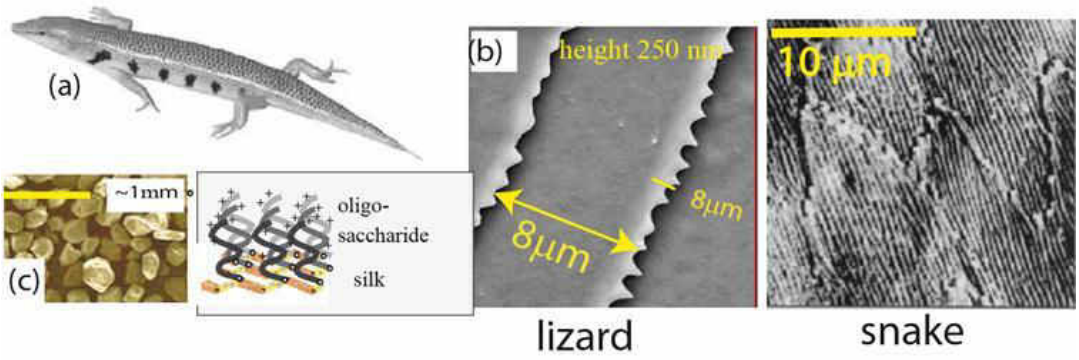


Figure 2: *Some remarkable features of sandfish. (a) Image of sandfish scincus albifasciatus. (b) Left: Surface profile of skin (Oberhäutchen) of lizard (scincus albifasciatus) exposing comb like protrusions on the back but not the belly. Right: Surface profile of snake skin which is made up of parallel ¬ β-¯ keratin bundles (silk hairs) with the tips pointing to the back. (c) Left: particles of desert sand in comparison with the distance between combs. Right: schematic view of oligosaccharide-filaments coupled to plate of β-keratin to which oligosaccharide chains are coupled. The hairs are neutral but they could be charged during motion due to frictional electricity.*

The surface of the sandfish exhibits several remarkable and unique features [7]:

- The keratins contain a high amount of sulphur which is assumed to be responsible for the high elastic constant of the Oberhäutchen, but it does not contain hard inorganic material, such as silicates or lime as assumed occasionally.
- A unique feature of the β-keratin of sandfishes is the exposure of neutral Oligo-saccharide chains. Neutral sugar groups are coupled to serine side chains of the β -keratin which can, however, be charged by phosphorylation.
- Most remarkable is the repulsive force exerted by the skin on AFM tips composed of silicon-nitride with or without silicon oxide layers. This repulsion is the same on the back and the belly, showing that it is not due to some specific surface profile, such as the comb-like protrusions at the back. However, removal of the sugar side chains by enzymes results in strong stickiness, showing that the repulsion is mediated by the surface chemistry and most likely due to polymer

induced forces (see below).

- An important property, closely related to the glycosylation of the keratin layer is the astonishing resistance of the skin to abrasion which can be tested by treatment with sandblaster. Comparison with different metals revealed an astonishing strong resistance to abrasion. While steel showed remarkable abrasion effects after 10 hours of sandblasting the skin showed no remarkable effect after such a treatment [3].

Friction control by polymer brushes

The control of adhesion and friction between solids by polymer films is an intensively studied field of biomimetic research. Natures made full use of this trick at all levels of organization. Without constant lubrication of the gap between moving joints of our body we cannot move, as people with Arthritis know well. Our knee joints are typically subjected to pressures of 5 MPa. In joints, the friction is reduced by the glycoprotein lubricin (with a molecular weight of ~230 kDa and a contour length Lc ≈ 200 nm) forming a composite gel with hyaluronic acid (see [8]). The gel is coupled to a layer collagen which forms an interface between the bone and the gel. The analogy with the structure of the sandfish skin shows first, that the concept of frictional reduction by polymer films was invented by nature long before the advent of mammalians and second, that nature uses the successful concept again and again.

The detailed molecular composition of the oligosaccharides of sandfish is not known yet, but their effect on friction has been well studied. For this purpose the skin is fixed on a glass plate tilted with respect to the horizontal by an angle α. Then a layer of sand is deposited on the surface. By measuring the maximum angle above which the sand start to slide one obtains the frictional coefficient μ_f, which is defined as the ratio of the frictional force F_p parallel to and the normal force F_n perpendicular to the plate (see [8]):

$$\mu_f = \frac{F_n}{F_n} = \tan \alpha_c$$

The critical angle is 21° for sandfish skin, 29° for glass and 36° for Teflon, that is the sandfish skin is a muchbetter frictional reducer than Teflon. Surprisingly the friction is the same at the back and belly of the sandfish despite of the lack of the comb structure on the latter [7]. A possible function of the comb-shaped protrusions on the back is to minimize the contact area with large sand corns at the back in order to compensate for the gravity.

Consider now a lizard swimming 10 cm below the surface. The pressure exerted on the back is p≈ 1600 Pa for a specific weight of 1.6 g cm^{-3} which would correspond to a strong frictional force. The sand particle exhibits diameter of about 0.5 mm and thus covers about 10 combs which would reduce the friction drastically, provided the polymer film is stable enough, a question discusses below.

***Polymer-induced repulsion forces*:** We have to consider two situations. First, surfaces covered by polymers that are separated by distances larger than their radius of gyration and second, surfaces covered by brush like assemblies of polymers.

In the first case the interaction between the polymer film and the sand particles can be described by the Dolan-Edwards potential, provided the separation between polymers is slightly larger than the radius of gyration R_g [13].

$$V_{rep}(h, R_g) \approx k_B T \rho_0 \left(\frac{R_g}{h}\right)^2 \exp\left[-\frac{3}{2}\left(\frac{h}{R_g}\right)^2\right]$$

Here ρ is the lateral density of the polymer chains. This equation holds below or near the overlap concentration $\rho R_g \leq 1$. The disjoining pressure is of the order of $p_{disj} \approx V_{rep}(h, R_g)/h$. To gain some insight into the strength of the disjoining pressure we consider an oligosaccharide chain with R_g≈ 10nm and assume that $\rho_0 \approx R_g^{-2}$. The repulsive pressure is:

$$p_{disj} = V_{rep}(h, R_g)/h \approx k_B T \exp\left\{-h/R_g\right\}^2.$$

Consider first the pressure of 10 cm thick layer of sand (specific weight 1.2 $grcm^{-3}$. The

gravitational pressure is 10 N.

To consider the question whether the Donna-Edwad Potential can resits the pressure of the10 cm thick sand layer. We assume for the polymer density $\rho_0 \approx R_g^{-2}$ which correspond to a pressure of :

$$p_{disj} = V_{rep}(h, R_g)/h \approx k_B T \ \exp\left[-\frac{3}{2}\left(\frac{h}{R_g}\right)^2\right] \approx 10^{-4} \exp\left\{\frac{R_g}{h}\right\}^2 Pa$$

To resist the sand pressure the ratio R_g/h must be of the order of $R_g/h \sim 10$. This shows that the polymer film will be completely compressed.

Clearly, to avoid complete compression the polymer density must be high with $\rho_0 > R_g^{-2}$.Under this condition the polymer forms soft elastic brushes. The Young moduli of polymer brushes of polyethylene is of the order of 10^6 Pa [14]. The compression of the hairy rods is thus very small (about $\delta h/h \approx G^{-1} p_{disj} \approx 10^{-5}$ =).The main advantage of layers of polymer brushes is the dissipation of energy by the high damping factor of polymerfilms.

Friction electricity may help the repulsion by hair raising effect. Owing to the low humidity of the desert the friction between sand and the skin of the lizzard results in high electric charging of the silk like surface [2, 7]. It has been speculated that the magnetic field generated by the moving animal might generate a repulsive force and reduce friction. However, the force would be too weak to lift sand particles form the surface against gravity. A more likely effect of the charging could be the stretching of the oligosaccharide filaments coupled to the keratin filaments. It is well known that the persistence length of polyelectrolytes is much larger than that of neutral macromolecules. In air the stretching effect would be larger since the charges are not screened by water molecules.

Acknowledgements: The work was supported by the Exzellenzinitiative "Emeriti of excellence" of the Technische Universität München and by the Lehrstuhl fuer Angewandte Physik (Professor Hermann Gaub) of the University of Munich.

References

[1] Sackmann, E. (2013) Biomimetic physics: learning from nature's strategies of overcoming evolutionary crises Int. J. Nanotechnology, Vol. 10, 376-389.

[2] Weiss, I., Lüke, F., Eichner, N., et al.(2013) On the function of chitin synthase extracellular domains in biomineralization. J. Structural Biology, 2013, 216-25.

[3] Rechenberg, I., et al. (2009) Schlußbericht BMBF Projekt F- 0311967A.

[4] Maladen, RD. et al (2011) Undulatory swimming in sand: experimental and simulation studies of a robotic sandfish. Internat. J. Robotics Research 30: 793-804.

[5] Taylor G, (1951'Analysis of swimming microorganisms', Royal Soc. London. Proc. Series A, 209, 447-461. (1951)

[6] Landau L. and Lifshitz E. Fluid Mechanics (Volume 6 of A Course of Theoretical Physics) Pergamon Press 1959.

[7] (a) Baumgartner, W. et al. (2007) The Sandfish's skin: morphology, chemistry and reconstruction. J. Bionic Engineering 4**,** 1-9. (b) Baumgartner, W. et al. (2008) Investigating the locomotion of the sandfish in desert sand using NMR-imaging. PLoS ONE Vol. 3, e3309.

[8] Jay G. (2007) Association between friction and wear in diarthrodial joints lacking lubricin Arthritis Rheum. Vol. 56, 3662–3669.

[9] Lee J and Herrmann H (1993) Angle of repose and angle of marginal stability: molecular dynamics of granular particles. J. of Physics A 26, 373–383.

[10] Ding, Y., Gravish, N. and. Goldman D. (2011) Drag induced lift in granular media. Phys Rev. Letter 106, 028001 -4

[11] Hazel, J., Stone M, Grace M., and Tsukruk V. (1999) Nanodesign of snake skin for reptation locomotions via frictional anisotropy. J of Biomechanics. 32, 477-484.

[12] Raviv, U., Giasson, S., Kampf, N., et al. (2003) Lubrication by charged polymers. Nature 245, 163-166.

[13] Bruinsma, R., Berisch, A., and Sackmann, E., (2000) Adhesive switching of membranes: Experiment and theory. Phys. Rev E. 61, 4253-4267.

[14] Prucker, O. et al.(1997) Swelling of a Polymer Brush Probed with a Quartz Crystal Resonator Phys. Rev. E 56, 680 –690.

Nanoglasses: A Way of alloying Materials that are immiscible in all of Today's Materials?

by Herbert Gleiter, Member EUAS

Short Biography

Institute of Nanotechnology, Research Center Karlsruhe, Germany

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

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

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

Abstract

Today's technologies are primarily based on crystalline materials (metals, semiconductors, etc.), as their properties can be controlled by varying their chemical and/or defect microstructures. This is not possible in today's glasses. The three new features of nanoglasses - consisting of nanometer-sized glassy regions connected by interfaces – are that (1) their properties may be controlled by varying their chemical and/ or (2) defect microstructures, and (3) that their interfaces have a non-crystalline structure that is different from the glassy structures known today. By utilizing these new features, an age of new technologies based on nanoglasses (a "glass age") may be initiated. This paper focuses on the following new perspective of nanoglasses: the perspective that nanoglasses permit the alloying of materials that are immiscible in all of today's materials**.**

Introduction and Basic Ideas

The history of mankind is intimately related to the materials available to create the tools required for developing new technologies. In fact, if the materials are considered that were used between the early days of the neolithicum (up to 80 000 years ago) and today, it may be seen that most of them have been crystalline materials. The main reason for the predominance of crystalline materials in the development of mankind is the fact that one

can control their properties by modifying their defect microstructures and/or their chemical microstructures. An example [1] is displayed in Figure 1.

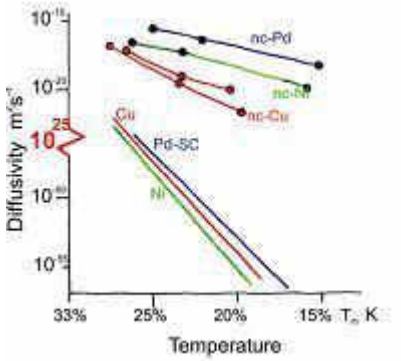


Figure 1 Comparison of the diffusivities in nanocrystalline (nc) Cu, Ni, and Pd as a function of temperature, relative to the diffusivities in single crystals (SC) of Cu, Ni, and Pd. Tm is the absolute melting temperature of Cu, Ni, and Pd.

Figure 1 shows the enhancement of the diffusivity by about thirty orders of magnitude due to the introduction of intercrystalline interfaces i.e. by changing their defect microstructure. Similarly, an example for the modification of the properties of crystalline materials by varying their chemical microstructures are shown [1] in Figure 2

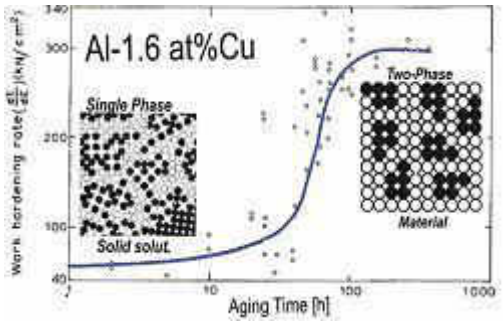


Figure 2 Work hardening rate of Al-1.6 at% Cu crystals at ambient temperature after a solution treatment followed by ageing at 190 °C for various times, as indicated on the horizontal axis.. The strain rate of the deformation process was 3 $\cdot 10^{-4}$ sec^{-1}. Initially the specimens were Al–Cu solid solutions, as is indicated schematically by the inserted drawing on the left side of the figure. The ageing at 190 °C resulted in the formation of a two-phase material consisting of crystalline precipitates embedded in a crystalline matrix, as indicated schematically by the inserted drawing on the right side of the figure. This variation of the chemical microstructure resulted in an increase of the work hardening.

by means of the work hardening rate of Al-1.6at% Cu crystals after a solution treatment followed by an ageing process at 190 °C for different times. Initially, the specimens were Al–Cu solid solutions, as is indicated schematically on the left side of Figure 2. Ageing at 190 °C resulted in the formation of a two-phase material consisting of crystalline precipitates embedded in a crystalline matrix, as indicated on the right side of Figure 2.

Glassy materials, although known for more than 10 000 years (e.g. in the form of obsidian), have not been utilized so far in a comparable large variety of technologies. The most important applications seem to be windows, lenses, optical fibers, amorphous magnets, and surface coatings. The main reason for this less frequent use of glasses is that they are mostly produced by quenching the melt and/or the vapor.

As today's glasses are produced most frequently by quenching the melt, the atomic structures of such glasses are essentially controlled by the structure of the molten state at

the glass transition temperature (T_g). This production process does not permit the introduction into glasses of defects that are, for example, similar to grain boundaries in crystalline materials (cf. Figure 3c). As a consequence, one cannot control the properties of the glasses we have today by the controlled modification of their defect and/or chemical microstructures, as was displayed in Figures 1 and 2 for crystalline materials.

However, the history of mankind teaches us that it is this controlled modification of the defect and/or chemical microstructures of materials that has opened in the past the way to new technologies. Hence, the door to a world of new technologies (beyond today's technologies based predominantly on crystalline materials) may be opened if one succeeds in synthesizing noncrystalline materials with controllable modification of their defect and/or chemical microstructures, called today nanoglasses. Nanoglasses, which will be discussed in this article, seem to represent a first attempt to open this door. Nanoglasses are based on the idea of applying analogous approaches for generating glasses with controllable defect microstructures or chemical microstructures in the form of interfaces between adjacent glassy regions with identical or with different chemical compositions.

If we start from a melt consisting of one kind of atom only (Figure 3e), we obtain (at least in principle) a glass by quenching the melt with a sufficiently high cooling rate (Figure 3 f). By analogy to Figure 3 c, it is proposed to introduce a high density of glass–glass interfaces by consolidating nanometer-sized glassy clusters (Figure 3 g) with identical or different (Figure 3h) chemical composition

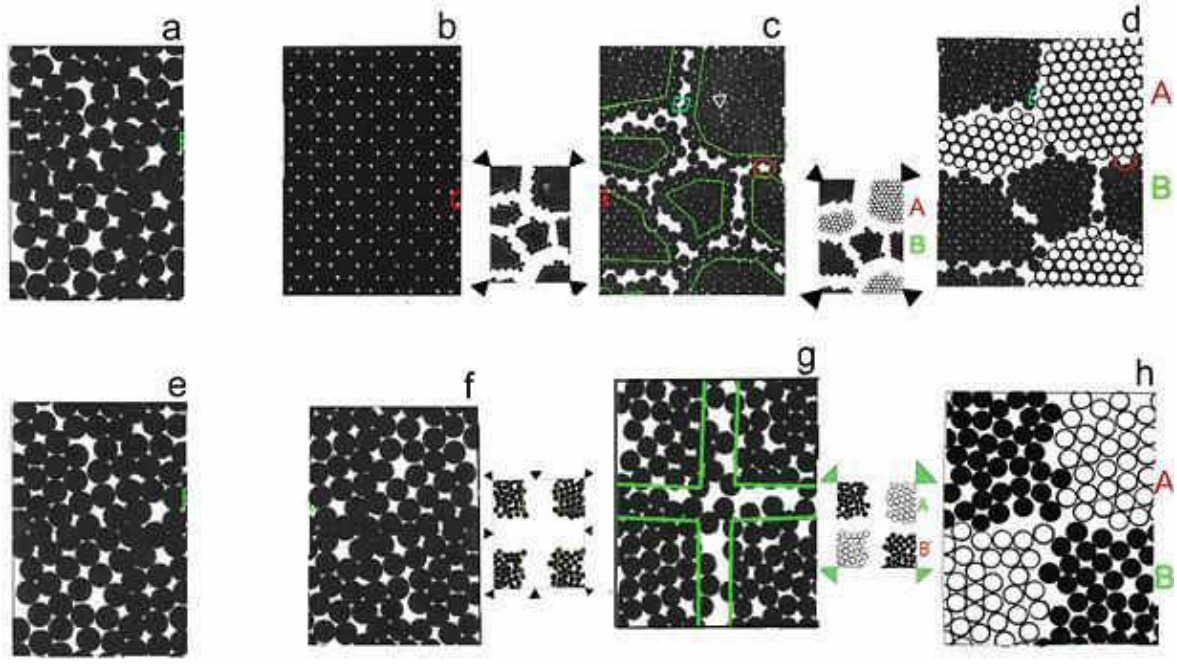


Figure 3. The analogy between the defect and the chemical microstructure of nanocrystalline materials (upper row of fi gures) and of nanoglassesm(lower row of figures). The defect microstructure in panel (c) and the chemical microstructure of a nanocrystalline material in panel (d) are comparedmin panels (g) and (h) with the corresponding defect microstructure and the corresponding chemical microstructure of a nanoglass.

In this paper we will focus on nanoglasses produced by consolidating nanometer–sized glassy clusters of different chemical compositions: called today multicomponent nanoglasses [1-4]. The novel aspect of these multicomponent nanoglasses is that they seem to permit the alloying of materials that are immiscible in all of today's materials and hence that may result in a new world of materials with new properties.

Multicomponent Nanoglasses: Noncrystalline Solids with New Chemical Microstructures

As was indicated in Figure 3 h, one way to produce multicomponent nanoglasses involves the consolidation of nanometer-sized glassy clusters with different chemical compositions. Studies by means of transmission electron microscopy (TEM) of a multiphase nanoglass [1-4] consisting of Fe 90 Sc 10 and Cu 64 Sc 36 glassy clusters confirmed the expected microstructure (Figures 3 g and h).

If these nanoglasses were annealed below the T_g of both components (e.g., for 3 h at 100 °C), a noncrystalline solid solution was formed (Figure 4 c), with a chemical composition of Fe 45 Sc 23 Cu 32. The uniform spatial distribution of Cu and Fe is remarkable because Fe and Cu are practically immiscible in the crystalline state. The formation of the solid solution shown in Figure 4 d may be understood, however, in terms of the noncrystalline structure of the clusters (Figure 4 a) as follows: the atomic arrangement in these clusters is the atomic arrangement of the melt that is frozen at the *T* g . Moreover,

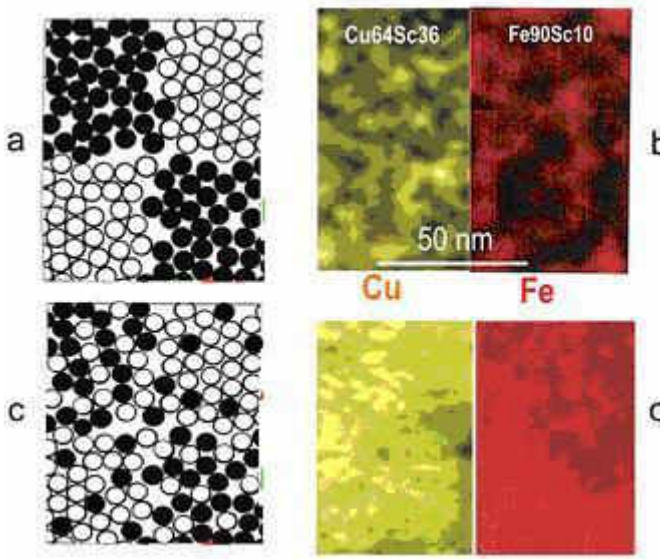


Figure 4. a) Hard sphere model of a nanoglass consisting of two glassy clusters with different chemical compositions. The two kinds of atoms forming the chemically different clusters are indicated by means of black and open circles. b) Compositional mapping (STEM image) of the Cu and the Fe distribution in an as-consolidated nanoglass, produced by consolidating glassy clusters with a chemical composition of Cu 64 Sc 36 and regions with a composition of Fe 90 Sc 10 . The spatial distribution of Cu and Fe in the as-consolidated nanoglass is indicated by yellow and red, respectively. Intensive yellow or red indicate high local concentrations of Cu or Fe, respectively. c) Hard sphere model of the nanoglass (shown in panel (a)) after annealing. During annealing, the two kinds of atoms interdiffuse, forming a noncrystalline solid solution with a uniform chemical composition. d) Compositional,mapping (STEM) of Fe and Cu in the nanoglass shown in panel (b) after annealing for at 3 h at 100 °C. As may be seen, the annealing has resulted in a spatially uniform distribution of the two alloy elements (Cu and Fe) [3].

it is known that Fe and Cu are miscible in the molten state. Hence if the structures of the glassy clusters (Figure 4 a) are similar to the structures of the corresponding melts (at *T* g), it may be expected that Fe and Cu are miscible in the glassy clusters as well. In terms of this interpretation, the observed enhanced miscibility should not be limited to Fe and Cu. In other words, multicomponent nanoglasses seem to open the way to generate alloys of components that are miscible in the molten state but not in the crystalline state. In fact, this may apply even if these clusters differ in terms of the nature of their chemical bonds, such as noncrystalline solid solutions of Fe–Si, Cu–Se, Fe–Ge, Cu–He, or Fe–H. One well

known example of this type is gold–ruby glasses produced by dissolving gold salts in molten SiO 2 [4].

Perspectives: New Technologies Based on Nanoglasses

The reported observations [1-4] about the new atomic as well as the new electronic structures of nanoglasses explain why the properties of nanoglasses differ from the properties of the glasses available today. Moreover, as was pointed out, it is these new atomic and electronic structures of nanoglasses that permit the modification of the properties of nanoglasses by essentially the same methods that were utilized for several thousands of years in the case of crystalline materials. Hence, new prospects for nanoglasses suggest that they may permit the utilization of noncrystalline materials in a comparable large variety of technological applications that were possible so far only in the case of crystalline materials [4]. By analogy to the importance of crystalline materials for most technological developments, it seems conceivable that, in the future, the novel properties of nanoglasses may permit numerous new technological developments that are based on the novel features of this new class of materials. At the moment, the main barrier to the technological application of nanoglasses is the fact that no method seems presently available for the economic production of large quantities of nanoglasses. However, history teaches us that ingenious methods for producing particular materials can be developed within relatively short periods of time, if it becomes obvious that these materials are technologically attractive. A well-known example is Al. When Al was discovered, its price was comparable to the price of gold. Within a few decades, the interesting properties of Al motivated the development of its electrolytic production, which reduced the price of Al to today's level. Hence, based on this experience, the present expensive production methods of nanoglasses, preventing their technological use, may be removed if more properties of nanoglasses are discovered that appear technologically attractive. If this were the case, it might be the first step toward what might finally develop into a "glass age".

References

[1] H.Gleiter, Th.Schimmel, H.Hahn, Nano Today **9** (2014) 17-68.
[2] Na Chen , X.Shi, R.Witte, K.Nakayama, K.Ohmura, H.Wu, A.Takeuchi, H.Hahn, M. Esashi, H. Gleiter, A. Inoue, D.Louzguine, J.Mater. Chem.**B1**, 2013 2568.
[3] Na Chen, Di wang, R.Feng, R. Kruk, Ke-Fu Yao, D. Louzguine, H. Hahn, H. Gleiter, Nanoscale **7,** 2015, 6607- 6611.
[4] H.Gleiter, Small **12** , 2016, 2225 – 2233.

Innovative Research in Plasticity Engineering

by Michael Kassner, Member EUAS

Short Biography

Choong Hoon Cho Chair and Professor University of Southern California

Michael Kassner graduated with a Bachelors in Science-Engineering from Northwestern University in 1972, and M.S. in Metallurgical Engineering at Illinois Inst. Tech. and an M.S. and Ph.D. inMaterials Science and Engineering from Stanford University in 1979 and 1981.

Kassner accepted a position at Lawrence Livermore National Laboratory in 1981 and was employed there until 1990. During that period he performed basic research on the mechanical behavior of metals, as well as a variety of defense-related projects. He was promoted to Head of the Physical Metallurgy and Welding Section and was the Thrust Leader for Physical Metallurgy Research. In 1984 he spent a year on leave at the Univ. of Groningen in The Netherlands as a Fulbright Senior Scholar.

Kassner accepted a faculty position in the Mechanical Engineering Department at Oregon State University in 1990 where he was Northwest Aluminum Professor of Mechanical Engineering and Director of the interdisciplinary PhD program in materials science. He received the College of Engineering Outstanding Sustained Research Award in 1995. While at Oregon State, Professor Kassner was detailed to Basic Energy Sciences of the U.S. Department of Energy and a Program Manager. He was also on leave for one year at the NSF Institute of Mechanics and Materials at the University of California at San Diego, where he was an Adjunct Professor. Prof. Kassner moved in 2003 to accept a position as Chairman, Mechanical and Aerospace Engineering Department ant the University of Southern California (USC). He is also a Professor of Materials Science at USC. He is currently Choong Hoon Cho Chair and Professor. Prof. Kassner is currently active in pursuing research at USC on creep, fracture, fatigue and thermodynamics.

Most recently, Prof. Michael Kassner was assigned to Washington D.C. as the Director of Research at the Office of Naval Research (ONR). He assumed the position in Oct. 2009. Until Oct. 2012. He was responsible for overseeing the nearly one billion dollar basic-research budget for the US Navy. He was awarded the Navy's Meritorious Public Service Medal for his tenure at ONR.

Prof. Kassner has published three books, one on the fundamentals of creep plasticity in metals, hot deformation of aluminum and aluminum alloys and another on phase diagrams and has authored or co-authored over 220 published articles. He serves on several editorial and review boards for major scientific journals. He is a Fellow of American Society of Metals (ASM), a Fellow of the American Society of Mechanical Engineers (ASME) and a Fellow of the American Assoc. for the Advancement of Science (AAAS).

M.E. Kassner

Fundamentals of Creep in Metals and Alloys 3rd Edition

Butterworth-Heinemann, 2015

Publisher Summary

Creep of materials is classically associated with time-dependent plasticity under a fixed stress at an elevated temperature. This chapter describes the plasticity under these conditions for constant stress and constant strain-rate conditions. The term "creep" as applied to plasticity of materials likely arose from the observation that at modest and constant stress, at or even below the macroscopic yield creep stress of the metal (at a "conventional" strain-rate), plastic deformation occurs over time. Stage I, or primary creep, denotes that portion where the creep-rate (plastic strain-rate) is changing with increasing plastic strain or time. The primary creep-rate decreases with increasing strain, but with some types of creep, such as solute drag with "3-power creep," an "inverted" primary occurs where the strain-rate increases with strain. Analogously, under constant strain-rate conditions, the metal hardens, resulting in increasing flow stresses. Often, in pure metals, the strain-rate decreases or the stress increases to a value that is constant over a range of strain. The phenomenon is termed Stage II, secondary, or steady-state creep. Eventually, cavitation and/or cracking increase the apparent strain-rate or decrease the flow stress. This regime is termed Stage III, or tertiary creep, and leads to fracture. Sometimes, Stage I leads directly to Stage III and an "inflection" is observed.

M.E. Kassner
The Dislocation Microstructure of Aluminum
Metallurgical and Materials Transactions A, 1987, Vol. 18, Issue 5, pp 835–846

Abstract
Aluminum of 99.999 pct purity was deformed in torsion at 644 K and an equivalent uniaxial strain rate of 5.04×10^{-4} s^{-1} to various steady-state strains up to 16.33. The subgrain size and density of dislocations not associated with subgrain boundaries remained fixed throughout the wide steady-state strain range. The subgrain boundaries, however, underwent two important changes. At the onset of steady state ($\varepsilon \sim 0.2$) all of the subgrain boundaries had relatively small misorientation angles averaging about 0.5 deg. With increased strain, however, an increasing fraction of the subgrain facets were high-angle boundaries. At strains greater than about four nearly a third of the boundaries were high-angle. In specimens with both types of boundaries, the high-angle boundaries have misorientation angles (θ) greater than 10 deg, while θ for low-angle boundaries is nearly always less than 3 deg. Only rarely do subgrain boundaries have misorientation angles between 3 deg and 10 deg. In aluminum, the increased high-angle boundary area at larger strains originates from the extension of the initial boundaries through the mechanism, recently introduced by others, of "geometric dynamic recrystallization" in aluminum. The average misorientation across low-angle boundaries initially increases during steady state but eventually reaches a maximum value of about 1.2 deg at $\varepsilon \simeq 1.2$. Since the flow stress stays nearly constant, the dramatic changes in the character of the subgrain boundaries that are observed during steady state suggest that the details of the boundaries arenot an important consideration in the rate-controlling process for creep.

L.E. Levine, B.C. Larson, W. Yang, M.E. Kassner et al.

X-ray microbeam measurements of individual dislocation cell elastic strains in deformed single-crystal copper

Nature Materials 5, 619–622 (2006)

The distribution of elastic strains (and thus stresses) at the submicrometre length scale within deformed metal single crystals has remarkably broad implications for our understanding of important physical phenomena. These include the evolution of the complex dislocation structures that govern mechanical behaviour within individual grains1, , the transport of dislocations through such structures, changes in mechanical properties that occur during reverse loading (for example, sheet-metal forming and fatigue), and the analyses of diffraction line profiles for microstructural studies of these phenomena. We present the first direct, spatially resolved measurements of the elastic strains within individual dislocation cells in copper single crystals deformed in tension and compression along 〈001〉 axes. Broad distributions of elastic strains are found, with important implications for theories of dislocation structure evolution3, dislocation transport, and the extraction of dislocation parameters from X-ray line profiles.

Texture, Microstructure and Mechanical Properties of Equiaxed Ultrafine-grained Zr Fabricated by Accumulative Roll Bonding

L. Jiang, M.T. Perez-Prado, P.A. Gruber, E. Artz, O.A. Ruano, M.E. Kassner
Acta Materialia , 2008, 56 (6), 1228-1242

Abstract

The texture, microstructure and mechanical behavior of bulk ultrafine-grained (ufg) Zr fabricated by accumulative roll bonding (ARB) is investigated by electron backscatter diffraction, transmission electron microscopy and mechanical testing. A reasonably homogeneous and equiaxed ufg structure, with a large fraction of high angle boundaries (HABs, ~ 70%), can be obtained in Zr after only two ARB cycles. The average grain size, counting only HABs ($\theta > 15°$), is 400 nm. (Sub)grain size is equal to 320 nm. The yield stress and UTS values are nearly double those from conventionally processed Zr with only a slight loss of ductility. Optimum processing conditions include large thickness reductions per pass ($\varepsilon \sim 75\%$), which enhance grain refinement, and a rolling temperature ($T \sim 0.3T_m$) at which a sufficient number of slip modes are activated, with an absence of significant grain growth. Grain refinement takes place by geometrical thinning and grain subdivision by the formation of geometrically necessary boundaries. The formation of equiaxed grains by geometric dynamic recrystallization is facilitated by enhanced diffusion due to adiabatic heating.

Neutron Reflectivity of Spintronic Materials

by Hartmut Zabel, Member EUAS

Short Biography

Education/Degrees:

1969 Bachelor in Physics, University of Bonn
1973 Master in Physics, Technical University of Munich
1978 Ph.D. in Physics, University of Munich

Academic Positions:

1978 - 1979 Postdoctoral Fellow, Department of Physics, University of Houston, Texas
1979 - 1983 Assistant Professor of Physics, University of Illinois at Urbana - Champaign
1983 - 1986 Associate Professor of Physics, University of Illinois at U - C
1986 - 1989 Professor of Physics, University of Illinois at U - C
1989 - 2013 Chair, Professor of Experimental Physics/Solid State Physics, Ruhr-Universität Bochum
2013 – 2019 Visiting Senior Research Professor, University of Mainz
since 1.4.1989 Adjunct Professor of Physics, University of Illinois at U - C

Guest positions:

Summer Guest Scientist, Brookhaven National Laboratory, 1985 and 1988; Guest Scientist, Risø National Laboratory, Denmark, 1986; Guest Scientist of the NIST, Reactor Division, Gaithersburg, USA, 1993; Guest Scientist of the Institut Laue-Langevin, Grenoble, France, 1997; Guest Scientist and Lecturer, University of Uppsala and KTH Stockholm, Sweden, 1998/99; Senior Guest Research Professor, University of Mainz, Germany, since 2013.

Fellowships/Awards:

Fellow of the Cusanus Fellowship Program for Superior Students, 1971 – 1973; Fellow of the Institute for Advanced Studies, University of Illinois at Urbana-Champaign, 1982; Fellow of the JSPS, 1989; Fellow of the Volkswagenstiftung, 1993 and 1997; Election to Fellow of the APS, 1996; Honorary Doctor of the KTH Stockholm, 2001; Elected "Outstanding Referee" of the APS, 2010; MAINZ Research Award, J G University Mainz, 2013; Elected Member, European Academy of Sciences, 2017.

Research Networks, Panels, and Advisory Committees:

Department of Energy (DOE) Program Director in the Materials Research Laboratory for the Condensed Matter Science Program (1986 – 1989); Member of the US DOE review panel "HFBR - Neutron Beam Lines" (1988); Member, Basic Energy Sciences Advisory Committee of the US DOE (1992); Chair, German – Russian Collaboration "Advanced Materials with Collective Electronic Properties", funded through the DFG and the Russian Academy of Science (1992-2002); Chairman of the DFG Collaborative Research Center "Magnetic Heterostructures: spin structure and spin transport" (2000-2011); International Advisor of the project "Fundamental Research and Applications of Magnetism" University of Uppsala (2001-2006); Chairman, Scientific Council of the Swiss Intense Neutron Source (SINQ) (2003-2005); Member, Beam time committee, BESSY Synchrotron facility, Berlin (2005-2012); Member and Chair of the Scientific Council, Institut Laue-Langevin, Grenoble (2006-2010); Member, Scientific Advisory Committee of the Hahn-Meitner Institut, Berlin (2004-2008); Divisional Associate Editor of the journal Physical Review Letters, (2012-2018); etc.

Further professional activities

Advisor of 50 PhD students with successful thesis completion, referee work for more than 25 journals, referee for more than 15 funding agencies, member of numerous national and international PhD disputation panels, organization of 4 international conferences and 4 summer schools, member of numerous advisory boards of national and international conferences, Chief Editor of the Elsevier Journal: Superlattices and Microstructures, Elsevier (2003-2013); etc.

Publications:

More than 500 refereed papers in technical journals, 36 review papers and book chapters, editor of five books , author of the textbook "Physik" , Thieme publisher, 1st edition 2011, 2nd edition 2016, author of the textbook "Medical Physics", de Gruyter publisher, 1st edition 2017.

Research activities:
Hydrogen in metals, graphite intercalation compounds, semiconductor heterostructures, metal superlattices and heterostructures, diffusion in solids, oxidation of epitaxial metal films, phase transitions, magnons, phonons, magnetism of thin films and heterostructures, proximity effects between superconductors and ferromagnets, spintronic materials, nanofluidics, magnetic x-ray and neutron scattering, magneto-optics. Spin-ice, magnetic nanoclusters, odd-triplett superconductivity; Most recently: time-resolved magnetization precession and magnetization reversal processes, antiferromagnetic spintronics.

Thermal neutron scattering is generally considered a bulk probe that is particularly sensitive to magnetic structures and magnetic excitations in solids. This is due to the fact that thermal neutrons have no electrical charge but a magnetic moment, their wavelength matches atomic distances in solids, and their energies are comparable to fundamental excitations such as phonons and magnons [1]. It is less well known that thermal or cold neutrons are, in addition, sensitive to magnetic surfaces and interfaces. This interface sensitivity turns out to be most useful in studies of magnetic thin films, multilayers, and lateral magnetic microstructures, which are of interest for spintronic applications [2]. The interface sensitivity is due to the wavelength (0.5-1.0 nm) of "cold" neutrons matching the thickness of thin films and to the distortion of the neutron wave field near surfaces when potential steps are encountered. This interface sensitivity is exploited in specular neutron reflectivity (NR) and in off-specular diffuse neutron scattering. The specular intensity (incident angle equals exit angle) yields information on the average film thickness and interface roughness, whereas the off-specular scattering (incident angle different from exit angle) is related to density fluctuations within the film plane [3].

When studying magnetic films and multilayers it is advantageous to first fix the neutron polarization, i.e. the neutron magnetic moment with respect to the scattering plane, and to analyze the polarization state of the exit beam before entering the detector. This variant of neutron reflectivity is called polarized neutron reflectivity (PNR), providing a highly sensitive measure of the strength and orientation of the magnetization vector within thin films. Therefore, PNR is also sometimes called a layer-resolving vector magnetometer. PNR has seen an upsurge of interest in recent years and a number of neutron reflectometers for magnetic studies have become available at all major steady state and pulsed neutron sources around the world [4]. Also, the European Spallation Source, presently under construction in Lund (Sweden), will be equipped with a polarized neutron reflectometer in the future [5]. Figure 1 shows the outline of the neutron reflectometer SuperADAM [6] installed at the research reactor of the Institut Laue-Langevin in Grenoble, France, for which the author was the project leader together with Professor B. Hjörvarsson of the Uppsala University, Sweden. Neutrons from a guide are reflected out by a graphite monochromator, selecting a fixed wavelength. The monochromatic neutron beam then passes a neutron spin polarizer and spin flipper before hitting the sample placed on a goniometer, and another neutron spin analyzer and spin flipper after reflection from the sample and before entering the detector. With this device, four different cross sections can be measured as a function of scattering angle: two spin conserving reflectivities for up and down polarized neutrons and two spin reversing reflectivities. These four reflectivities yield detailed information on the magnetic state in thin films and multilayers and how the magnetization changes when exposed to temperature and/or magnetic fields.

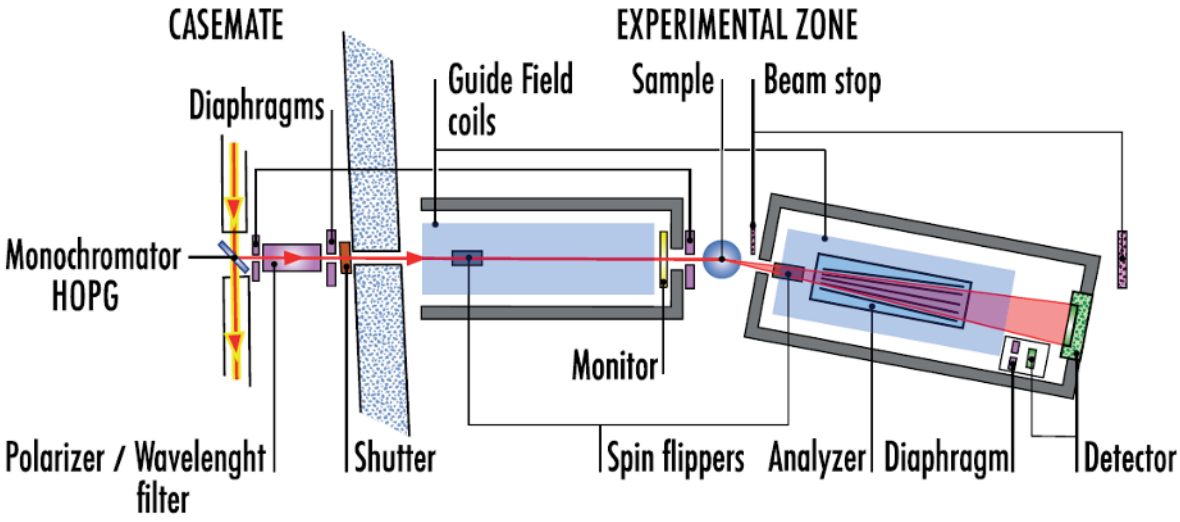


Figure 1: Schematic layout of the neutron reflectometer Super ADAM with polarization option, installed in the guide hall of the high flux neutron research reactor of the Institut Laue-Langevin in Grenoble, France. A broad band neutron beam enters through a neutron guide from the top left side. Neutrons with a specific wavelength are filtered out and deflected with the help of a graphite monochromator. Then they pass a polarizer, which keeps one neutron polarization (neutron spin orientation) and eliminates the opposite one. To avoid depolarization, the polarized and monochromatized neutron beam is kept in a magnetic guide field. Before hitting the sample, a spin flipper can switch the neutron beam polarization when activated. After the sample table, a second spin flipper is installed that can reverse the neutron spin again and together with a fan analyzer allows to determine the exit spin state even for a divergent and diffuse outgoing neutron beam. A position sensitive detector records concurrently the specularly reflected and the off-specularly scattered neutron beam. Reproduced from Ref. [6].

Our present-day knowledge of magnetic heterostructures has greatly benefited from various applications of PNR, detailed overviews are given in Ref. [7,8]. In particular, these include the determination of magnetization vectors and magnetic domain structures in artificial superlattices with collinear and non-colinear orientations; magnetization profiles and magnetization reversals in novel magnetic alloys and compounds; proximity effects in ferromagnetic/antiferromagnetic or ferromagnetic/superconducting heterostructures; phase transitions in ferro- and ferrimagnetic compounds with rare earth elements; and magnetization reversal processes in laterally patterned arrays of magnetic islands and stripes.

Lateral Magnetic Patterns

Presently there is a considerable activity in fabrication and characterization of lateral magnetic nanostructures [9]. This field is driven by a genuine and fundamental interest in magnetic properties on the nanoscale as well as by the large potential for applications in magneto-electronic and spintronic devices. The main questions concern (1) the spin structure in nano-patterned media as a function of the shape, size and separation of the islands; (2) the mechanism of reversal via coherent magnetization rotation or domain wall motion; (3) the speed of the reversal and the damping mechanism of spin excitations; (4) different methods for driving the reversal via an external field, spin accumulation, or

current torque; and (5) the bipolar stability of spin structure versus thermal fluctuations as a function of size and anisotropy of magnetic nanoparticles.

Neutron reflectivity from magnetic nanostructures is a challenging task. Nevertheless, it is worth pursuing it because of the unique information that this method offers for the understanding of correlation effects and magnetization fluctuations. The application of PNR requires fabrication of large arrays of magnetic elements to compensate for the small scattering volume. For laterally structured thin films with a defined periodicity, such as arrays of magnetic stripes, Bragg reflections occur in the scattering plane to left and to the right side of the the specularly reflected beam. Both the specular reflectivity and the Bragg peaks can be studied as a function of the external field for a detailed analysis of the reversal mechanism. An example is shown in Figure 2 taken from Ref. [11]. In this particular case, a multilayer was deposited on a magnesium-oxide substrate by sputtering methods with the layer sequence Cr/Fe/Cr/Co/Cr that was repeated 8 times. Such a multilayer produces Bragg peaks in the perpendicular direction (q_z) when x-rays or neutrons are reflected at specular conditions $\alpha_i = \alpha_f$. This is schematically shown in panel (a). However, with neutron reflectivity, we have, in addition, the option to record the reflected intensity for spin up (+) neutrons or spin down (-) neutrons. The difference of the reflected intensity, normalized by the sum is called asymmetry and is directly proportional to the magnetization profile in the q_z – direction.

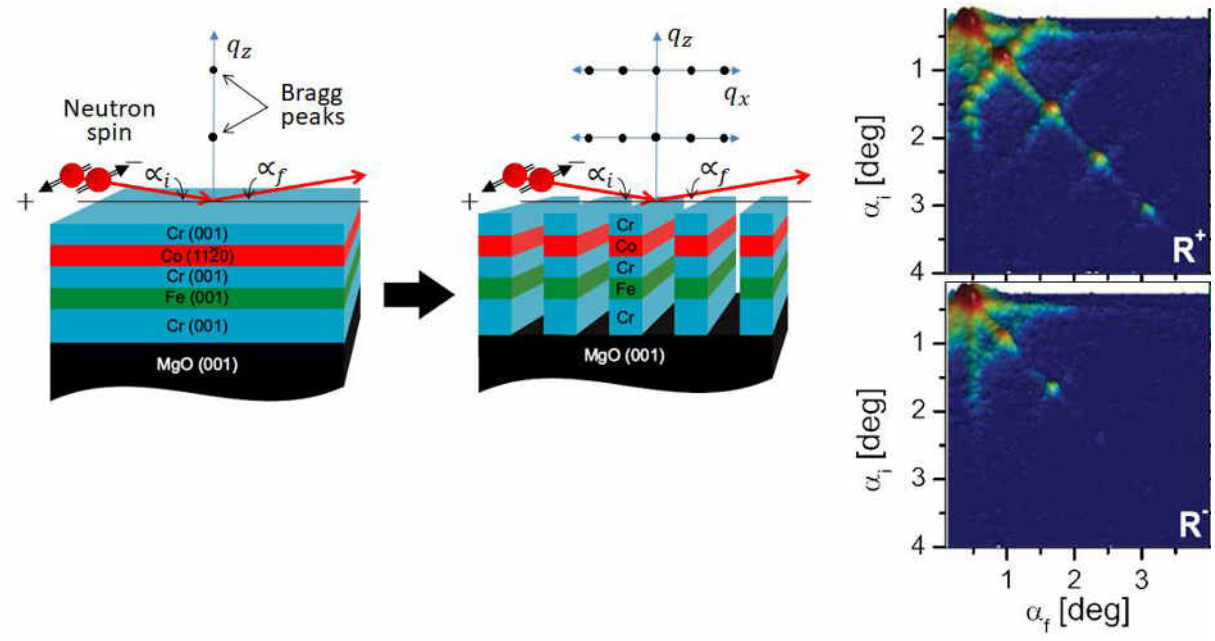


Figure 2: (a) Sequence of alternating magnetic and non-magnetic layers produced by sputtering methods on a MgO target. On top of the multilayer is schematically shown the scattering geometry for specularly reflected neutrons with spin up (+) and spin down (-) polarization. (b) The multilayer is laterally patterned by lithographic means into stripes of width 2 μm and stripe separation of 4 μm, yielding a lateral periodicity of 6 μm. The lateral periodicity gives rise to additional Bragg peaks in the q_x – direction. (c) Intensity maps recorded with up and down polarized neutrons from the lateral magnetic pattern. Note the intensity difference, which is due to the ferromagnetic state of the sample. Adapted from Ref. [11].

Next we study this multilayer after patterning by lithographic means, which produces a striped multilayer as shown in panel (b). Now we have two periodicities, one in the perpendicular direction and another one in the lateral direction. Accordingly, we expect Bragg reflections along q_z and q_x, which have again different intensities, when probed by polarized neutrons. The intensity maps in panel (c) for (+) and (-) polarized neutrons show all the expected features. Along the diagonal, which marks the specular condition $\alpha_i = \alpha_f$, we find the Bragg reflections from the periodicity in the perpendicular direction. In addition, many Bragg reflections are visible in the q_x – direction due to the lateral periodicity. Furthermore, a pronounced intensity difference can be seen in the maps recorded for up and down polarized neutrons, which is the hallmark of the ferromagnetic state of this multilayered and patterned heterostructure. When the magnetization is reversed in this striped multilayers, the stripes may interact via stray magnetic dipolar fields. PNR allows to identify these fields and to quantify to what extent the reversal becomes correlated in comparison to isolated stripes. Clearly, in a magnetic memory device, each magnetic island should be switchable as autonomous as possible. Furthermore, the lateral Bragg reflections indicate that the neutron coherence length must be considerably longer than the lateral periodicity of 6 μm. In fact, the coherence length of neutrons was, in the presented case, on the order of 50 μm.

This is but just one example of PNR applications to magneto-electronic/spintronic issues. Another hot topic, presently studied by several groups, is the self-organization of magnetic nanoparticles on solid or soft substrates [12,13]. Here the interest is to understand both, the interaction of the nanoparticles with the substrate and the magnetic dipole-dipole interaction among the nanoparticles. These studies will be extended to the investigation of magnetic nanoparticles interacting with relevant biological membranes or tissues. Diffusion processes through membrane channels as well as perfusion through leaking membranes need to be considered and can be analysed with methods described in this short communication.

Future Challenges and Opportunities

Neutron reflectivity of spintronic materials has proven in the past to be an crucial method for the analysis of domain structures in thin films, magnetic roughness at interfaces, correlation effects, and fluctuations. After many years of intensive developments of all aspects of polarized neutron reflectivity, including polarizers, spin-flipper, wide-angle spin analyzer, area detectors, etc. the main remaining challenges are sample size and intensity. They go hand in hand. Neutron reflectivity requires only about 1 μg of material. This is six orders of magnitude less than samples for typical bulk neutron scattering experiments and an amazing achievement so far. However, in the future the lateral sample size, i.e. scattering volume, needs to be further reduced and combined with external pertubations, such as laser pulses, a.c. magnetic fields, or current pulses for testing, in operando, functional response on the micro- to nanoscale. There is still much to do in the coming years.

We conclude by mentioning that in recent years competition to polarized neutron reflectivity has evolved from x-ray resonant magnetic scattering (XRMS) with soft x-rays [14,15]. The usually weak cross section for magnetic x-ray scattering is enhanced by resonant excitation of core levels with circularly polarized x-ray photons, making the method, in addition, element specific. Using XRMS methods with photon wavelengths

comparable to cold neutrons, the magnetization profile can be probed, element-specific magnetic hysteresis can be measured, ferro- and antiferromagnetic orderings in thin films and multilayers can be analyzed, and charge as well as orbital ordering effects can be detected. Nevertheless, there are distinct differences in PNR and XRMS methods that concern the selection rule for magnetic scattering and the spin-charge cross terms. In general and without going into further details, one may state that XRMS is a very powerful method, in particular for the investigation of nanomagnetic systems, but more difficult to analyze when retrieving absolute quantitative data as compared to PNR. In any case, it has become common practice nowadays to use both methods for a complete analysis of nanomagnetic systems.

References

1. S.W. Lovesey, "Theory of neutron scattering from condensed matter", Vol. 1 and 2, International Series of Monographs on Physics No 72, Clarendon Press, Oxford 1984.
2. S.D. Bader and S.S.P. Parkin, Annu. Rev. Condens. Matter Phys. 1:71–88 (2010).
3. C. Fermon, F. Ott, A. Menelle: *Neutron Reflectometry*. In: Jean Daillant, Alain Gibaud (Hrsg.): *X-ray and Neutron Reflectivity: Principles and Applications*. Springer, 2008.
4. http://www.reflectometry.net/reflect.htm#Theory
5. https://www.psi.ch/lns/estia
6. A. Devishvili, K. Zhernenkov, A. J. C. Dennison, B.P. Toperverg, M. Wolff, B. Hjörvarsson, and H. Zabel, Rev. Scientific Instrum. **84**, 025112 (2013)
7. H. Zabel, K. Theis-Bröhl, and B. P. Toperverg, In: The Handbook of Magnetism and Advanced Magnetic Materials, Vol. 3 - Novel Techniques, H. Kronmüller, S.P.S. Parkin (Eds.), Wiley, New York (2007), pp. 2327 - 2362
8. Boris P. Toperverg and Hartmut Zabel, Chapter 6 *Neutron Scattering in Nanomagnetism* in Neutron Scattering - Magnetic and Quantum Phenomena, Experimental Methods in the Physical Sciences, edited by Felix Fernandez-Alonso and David L. Price, Vol. 48, Academic Press (imprinted of Elsevier), 2015.
9. A. O. Adeyeye and N. Singh, J. Phys. D: Appl. Phys. 41, 153001 (2008).
10. Olav Hellwig, Laura J. Heyderman, Oleg Petracic, Hartmut Zabel, Springer Tracts in Modern Physics **246,** 189-234 (2013).
11. F. Brüssing, B. P. Toperverg, A. Devishvili, G. A. Badini Confalonieri, K. Theis-Bröhl, and H. Zabel, J. of Applied Physics **117**, 133903 (2015).
12. D. Mishra, O. Petracic, A. Devishvili, K. Theis-Bröhl, B. P. Toperverg and H. Zabel, J. Phys.: Condens. Matter 27, 136001 (2015) ***doi:10.1088/0953-8984/27/13/136001***
13. K. Theis-Broehl, E. C. Vreeland, A. Gomez, D. L Huber, A. Saini, M. Wolff, B. Maranville, E. Brok, K. L. Krycka, J. A. Dura, and J. A. Borchers, *ACS Appl. Mater. Interfaces*, Jan 2018
14. J. Fink, E. Schierle, E. Weschke and J. Geck, Rep. Prog. Phys. 76 056502 (2013).
15. S. Macke and E. Goering, J. Phys.: Condens. Matter 26 3632018 (2014).

Game Theory - Based Control System Algorithms with Real - Time Reinforcement Learning

by Frank Lewis, Member EUAS

Short Biography

F. L. Lewis, Ph.D., Fellow, National Academy of Inventors
UTA Research Institute - The University of Texas at Arlington
Fellow IEEE, Fellow IFAC, Fellow U.K. Inst. MC, Fellow AAAS
Professional Engineer Texas, Chartered Engineer U.K.
University Distinguished Scholar Professor, University Distinguished Teaching Professor
Moncrief-O'Donnell Endowed Chair, Head, Advanced Controls & Sensors Group
Qian Ren Thousand Talents Consulting Professor, Northeastern University, Shenyang, China.
Dr. Lewis was born in Würzburg, Germany, subsequently studying in Chile and Gordonstoun School in Scotland. He obtained the Bachelor's Degree in Physics/Electrical Engineering and the Master's of Electrical Engineering Degree at Rice University in 1971. He spent six years in the U.S. Navy, serving as Navigator aboard the frigate USS Trippe (FF-1075), and Executive Officer and Acting Commanding Officer aboard USS Salinan (ATF-161). In 1977 he received the Master's of Science in Aeronautical Engineering from the University of West Florida. In 1981 he obtained the Ph.D. degree at The Georgia Institute of Technology in Atlanta, where he was employed as a professor from 1981 to 1990. He is Moncrief-O'Donnell Endowed Chair Professor of Electrical Engineering at The University of Texas at Arlington.
Member, National Academy of Inventors. Fellow of the IEEE, Fellow of IFAC, Fellow of the U.K. Institute of Measurement & Control, Fellow American Association for the Advancement of Sciences, Member of the New York Academy of Sciences. Registered Professional Engineer in the State of Texas and Chartered Engineer, U.K. Engineering Council. Qian Ren Thousand Talents Consulting Professor, Northeastern University, Shenyang, China. Charter Member (2004) of the UTA Academy of Distinguished Scholars. UTA Academy of Distinguished Teachers 2012. IEEE Control Systems Society Distinguished Lecturer 2012-1014. Founding Member of the Board of Governors of the Mediterranean Control Association. Served as Visiting Professor at Democritus University in Greece, Hong Kong University of Science and Technology, Chinese University of Hong Kong, City University of Hong Kong, National University of Singapore, Nanyang Technological University Singapore. Distinguished Foreign Scholar, Nanjing Univ. Science & Technology. Project 111 Professor at Northeastern University, China. Elected Guest Consulting Professor at Shanghai Jiao Tong University and South China University of Technology.
Received IEEE Computational Intelligence Society Neural Networks Pioneer Award 2012, AIAA Intelligent Systems Award 2016. Received Fulbright Research Award 1988, American Society of Engineering Education F.E. Terman Award 1989, Int. Neural Network Soc. Gabor Award 2009, U.K. Inst Measurement & Control Honeywell Field Engineering Medal 2009, three Sigma Xi Research Awards, UTA Halliburton Engineering Research Award, UTA Distinguished Research Award, ARRI Patent Awards, various Best Paper Awards, IEEE Control Systems Society Best Chapter Award (as Founding Chairman of DFW Chapter), and National Sigma Xi Award for Outstanding Chapter (as President of UTA Chapter). Received Outstanding Service Award from the Dallas IEEE Section and selected as Engineer of the year by Ft. Worth IEEE Section. Listed in Ft. Worth Business Press Top 200 Leaders in Manufacturing. Appointed to NAE Committee on Space Station in 1995 and IEEE Control Systems Society Board of Governors in 1996. Received the 2010 IEEE Region 5 Outstanding Engineering Educator Award and the 2010 UTA Graduate Dean's Excellence in Doctoral Mentoring Award. Texas Regents Outstanding Teaching Award 2013.
Current interests include intelligent control, distributed cooperative control on graphs, nonlinear

systems, reinforcement learning, process control, condition-based maintenance, and neurobiological systems. Author of 7 U.S. patents, 354 journal papers, 52 chapters and encyclopedia articles, 416 refereed conference papers, and 20 books including Optimal Control, Optimal Estimation, Applied Optimal Control and Estimation, Aircraft Control and Simulation, Control of Robot Manipulators, Neural Network Control, High-Level Feedback Control with Neural Networks and the IEEE reprint volume Robot Control. Editor of Taylor & Francis Book Series on Automation & Control Engineering. Served as Editor for the flagship journal Automatica. Served/serves on many Editorial Boards including International Journal of Control, Neural Computing and Applications, Optimal Control & Methods, and Int. J. Intelligent Control Systems. Recipient of NSF Research Initiation Grant and continuously funded by NSF since 1982. Since 1991 he has received $8 million in funding from NSF, ARO, ONR, AFOSR and other government agencies, including significant DoD SBIR and industry funding. His SBIR program was instrumental in ARRI's receipt of the US SBA Tibbets Award in 1996.

Complex human-engineered systems involve an interconnection of multiple decision makers (or agents) whose collective behavior depends on a compilation of local decisions that are based on partial information about each other and the state of the environment [1]–[4]. Strategic interactions among agents in these systems can be modeled as a multiplayer simultaneous-move game [5]–[8]. The agents involved can have conflicting objectives, and it is natural to make decisions based upon optimizing individual payoffs or costs.

Game theory has been mostly pioneered in the field of economics; [9] considered a finite win-loss game with perfect information between two players, and this classic example of computable economics stands in the long and distinguished tradition of game theory that goes back to [10] and [11]. Reference [12] discusses game theory in algorithmic modes but not in what is today referred to as algorithmic game theory after realizing the futility of "algorithmizing" the uncompromisingly subjective von Neumann and Nash approach [13], [14] and beginning to understand the importance of Harrop's theorem [15].

Study in the control systems community has primarily focused on noncooperative zero-sum games arising in the form of H3 robust control of single-agent systems. Nonzerosum multiplayer game-theoretic control methods have also been employed to provide a basis for the study of coordination, conflict, and control for a single dynamical system with multiple players or control inputs. Graphical games [16] are also used for the case where players communicate using a graph network topology and can only receive information along the graph edges. Multiplayer games arise in real-world scenarios to find ways, for example, to optimally allocate the resources of optical networks [17], design optimal motion planning for multiple robots with different goals [18], study the coalition formation of robots for detecting intrusion [19], coordinate the charging of autonomous plug-in electric vehicles [20], design cooperative controllers across the electricity network to find new transmission routes when a power line is broken [21], [22], to protect a network from adversaries [23], [24], and provide behavioral decision-making models for planning and operating transportation systems [25].

Strategies for team decision problems, including *N*-player games (both nonzero sum and zero sum), are normally solved offline by solving the coupled Hamilton–Jacobi (HJ) equations for nonlinear systems or coupled Riccati equations for linear systems. For example, max-plus basis methods have been widely used to solve the HJ equations [26], [27]. This method employs grid-based methods, such as finite-difference or finite-element methods, to approximate the solution to the HJ equations. Although elegant, this approach is offline, requires complete knowledge of the system dynamics, and the computational time grows exponentially with the state-space dimension. Moreover, using these offline approaches, players cannot change their objectives online in real time without calling for a

completely new offline solution for the new strategies. However, given the nature of cooperation (or conflict) and that the environment is highly uncertain and dynamic, enabling autonomous agents to gracefully adapt their decision-making strategies to changes in the environment and in the behavior of the other agents is of paramount importance. As a learning technique that does not require a model of the environment and can be used online in real time, reinforcement learning (RL) is well suited for multiplayer games, where each agent knows little about other agents and the environment. Using RL, the agents can learn new behaviors online in real time, such that the performance of the individual or all players gradually improves. RL [28] is a subarea of machine learning concerned with how to methodically modify the actions of an agent (player) based on observed responses from its environment [29]–[33]. Two predecessors of the current article that focused only on single player games for optimal regulation of discrete-time systems are [31] and [34].

In game theory, RL is considered to be a bounded-rational interpretation of how equilibrium may arise. RL methods offer many advantages that have motivated control-systems researchers to develop RL algorithms that result in optimal feedback decision makers or controllers for dynamic systems described by difference equations or ordinary differential equations. These RL algorithms involve a computational-intelligence technique known as *policy iteration* (PI) [28], which refers to a class of two-step iteration algorithms: policy evaluation and policy improvement. PI provides an effective means to learn solutions to HJ equations online. In control-theoretic terms, the PI algorithm amounts to evaluating a policy by learning the solution to a nonlinear Lyapunov equation using generated data from a behavior policy and then updating the policy through minimizing a Hamiltonian function [35]. In on-policy RL algorithms, the policy being learned or evaluated is the same as the behavior policy being executed. In off-policy RL algorithms, on the other hand, the algorithm evaluates a policy or policies different from the one executed. Every decision maker tries to optimize its own objective defined in terms of the system dynamics. The actions by one decision maker will influence the actions of the other decision makers and will eventually lead to some kind of "negotiation."

The purpose of this article is to show how to solve multiplayer games online by adaptive learning in real time using data measured along the trajectories of the players. The full dynamics of the players do not need to be known for these online solution techniques. These methods implicitly solve the required game design equations without ever explicitly solving them. The algorithms are based on an actor/critic framework where the critic approximators are used to learn the optimal costs and the actor approximators are used to learn the optimal control policies. This article provides a truly dynamic framework for team decision making, since players or teams can change their objectives or optimality criteria on the fly, and the new strategies for all players, appropriate to the new situation, are then recomputed in real time. This online gaming approach also allows for timevarying team dynamics. It will be evident in networked systems that an agent affects the agents who are close enough to it. The team does better, in terms of achieving its goals, by using a distributed machine-learning approach that enables agents to exchange what they have learned.

References

[1] A. Rantzer. (2008, July). Using game theory for distributed control engineering, Tech. Rep., Dept. Automatic Control, Lund Univ., Sweden [Online]. Available: https://editorialexpress.com/cgi-bin/conference/

[2] J. R. Marden and J. S. Shamma, "Game theory and distributed control,"in *Handbook of Game Theory*, vol. 4, P. Young and S. Zamir, Eds. New York: Elsevier Science, 2014, pp. 816–900.

[3] E. Semsar-Kazerooni and K. Khorasani, "Multi-agent team cooperation: A game theory approach," *Automatica*, vol. 45, no. 10, pp. 2205–2213, 2009.
[4] F. L. Lewis, H. Zhang, K. Hengster-Movric, and A. Das, *Cooperative Control of Multi-Agent Systems: Optimal and Adaptive Design Approaches*. New York: Springer-Verlag, 2013.
[5] T. Basar and G. J. Olsder, *Dynamic Noncooperative Game Theory*. Philadelphia, PA: SIAM, 1995, vol. 200.
[6] W. B. Arthur, S. N. Durlauf, and D. A. Lane, *The Economy as an Evolving Complex System II*, vol. 28. Reading, MA: Addison-Wesley, 1997.
[7] C. Camerer, *Behavioral Game Theory: Experiments in Strategic Interaction*. Princeton, NJ: Princeton Univ. Press, 2003.
[8] J. Engwerda, *LQ Dynamic Optimization and Differential Games*. New York: Wiley, 2005.
[9] M. O. Rabin, "Effective computability of winning strategies," *Contrib.Theory Games*, vol. 3, no. 39, pp. 147–157, 1957.
[10] U. Schwalbe and P. Walker, "Zermelo and the early history of game theory," *Games Econ. Behav.*, vol. 34, no. 1, pp. 123–137, 2001.
[11] M. Euwe, M. Blaine, and J. Rumble, *The Logical Approach to Chess*. New York: Dover, 1958.
[12] K. V. Velupillai, "Non-linear dynamics, complexity and randomness: Algorithmic foundations," *J. Econ. Surv.*, vol. 25, no. 3, pp. 547–568, 2011.
[13] J. Von Neumann and O. Morgenstern, *Theory of Games and Economic Behavior*. Princeton, NJ: Princeton Univ. Press, 2007.
[14] J. Nash, "Non-cooperative games," *Ann. Math.*, vol. 54, no. 2, pp. 286–295, Sept. 1951.
[15] R. Harrop, "On the recursivity of finite sets," *Math. Logic Quart.*, vol. 7, no. 7–10, pp. 136–140, 1961.
[16] M. Kearns, "Graphical games," in *Algorithmic Game Theory*, vol. 3, N.Nisan, T. Roughgarden, E. Tardos. and V. Vazirani, Eds. Cambridge, U.K.: Cambridge Univ. Press 2007, pp. 159–180.
[17] L. Pavel, "A noncooperative game approach to OSNR optimization in optical networks," *IEEE Trans. Automat. Control*, vol. 51, no. 5, pp. 848–852, 2006.
[18] S. M. LaValle and S. Hutchinson, "Optimal motion planning for multiple robots having independent goals," *IEEE Trans. Robot. Automat.*, vol. 14, no. 6, pp. 912–925, 1998.
[19] X. Liang and Y. Xiao, "Studying bio-inspired coalition formation of robots for detecting intrusions using game theory," *IEEE Trans. Syst., Man, Cybern., Syst. B: Cybern.*, vol. 40, no. 3, pp. 683–693, 2010.
[20] Z. Ma, D. S. Callaway, and I. Hiskens, "Decentralized charging control of large populations of plug-in electric vehicles," *IEEE Trans. Control Syst. Technol.*, vol. 21, no. 1, pp. 67–78, 2013.
[21] W. Saad, Z. Han, H. V. Poor, and T. Bas‧ ar, "Game-theoretic methods for the smart grid: An overview of microgrid systems, demand-side management, and smart grid communications," *IEEE Signal Process. Mag.*, vol. 29, no. 5, pp. 86–105, 2012.
[22] A. B. MacKenzie and S. B. Wicker, "Game theory in communications: Motivation, explanation, and application to power control," in *Proc. Global Telecommunications Conf.,* 2001, vol. 2, pp. 821–826.
[23] T. Alpcan and T. Basar, *Network Security: A Decision and Game-TheoreticApproach*. Cambridge, U.K.: Cambridge Univ. Press, 2010.
[24] S. Roy, C. Ellis, S. Shiva, D. Dasgupta, V. Shandilya, and Q. Wu, "A survey of game theory as applied to network security," in *Proc. 43rd Hawaii Int. Conf. System Sciences*, 2010, pp. 1–10.
[25] C. Fisk, "Game theory and transportation systems modelling," *Transport. Res. B: Meth.*, vol. 18, no. 4, pp. 301–313, 1984.
[26] W. M. McEneaney, *Max-Plus Methods for Nonlinear Control and Estimation*. Boston, MA: Birkhauser, 2006.
[27] W. Fleming and W. M. McEneaney, "A max-plus-based algorithm for a Hamilton–Jacobi–Bellman equation of nonlinear filtering," *SIAM J. ControlOptim.*, vol. 38, no. 3, pp. 683–710, 2000.
[28] R. S. Sutton and A. G. Barto, *Reinforcement Learning: An Introduction*, vol. 1. Cambridge, MA: MIT Press, 1998.
[29] F. Lewis and D. Liu, *Reinforcement Learning and Approximate DynamicProgramming for Feedback Control* (IEEE Press Series on Computational Intelligence). New York: Wiley, 2013.
[30] K. Vamvoudakis, P. Antsaklis, W. Dixon, J. Hespanha, F. Lewis, H. Modares, and B. Kiumarsi, "Autonomy and machine intelligence in complex systems: A tutorial," in *Proc. American Control Conf.*, July 2015, pp. 5062–5079.
[31] F. L. Lewis, D. Vrabie, and K. G. Vamvoudakis, "Reinforcement learning and feedback control: Using natural decision methods to design optimal adaptive controllers," *IEEE Control Syst.*, vol. 32, no. 6, pp. 76–105, 2012.
[32] L. Busoniu, R. Babuska, B. De Schutter, and D. Ernst, *Reinforcement Learning and Dynamic Programming Using Function Approximators*, vol. 39. Boca Raton, FL: CRC, 2010.
[33] H. Zhang, D. Liu, Y. Luo, and D. Wang, *Adaptive Dynamic Programming for Control: Algorithms and Stability*. New York: Springer-Verlag, 2012.
[34] F. L. Lewis and D. Vrabie, "Reinforcement learning and adaptive dynamic programming for feedback control," *IEEE Circuits Syst. Mag.*, vol. 9, no. 3, pp. 32–50, 2009.
[35] D. Vrabie, K. Vamvoudakis, and F. Lewis, *Optimal Adaptive Control and Differential Games by Reinforcement Learning Principles*. *IET Control Engineering Series*. United Kingdom: Institution of Engineering and Technology, 2013.

Innovative Research in Alzheimer's Disease (AD)

by George Perry, Member EUAS

Short Biography

George Perry is dean of the College of Sciences, professor of biology and chemistry, and holds the Semmes Foundation Distinguished University Chair in Neurobiology at The University of Texas at San Antonio. Perry is recognized in the field of Alzheimer's disease research, particularly for his work on oxidative stress.

Perry received his Bachelor of Arts degree in zoology with high honors from University of California, Santa Barbara. After graduation, he headed to Scripps Institution of Oceanography, Hopkins Marine Station and Woods Hole, and obtained his Ph.D. in marine biology. He then received a postdoctoral fellowship in the Department of Cell Biology in the laboratories of Drs. Bill Brinkley and Joseph Bryan at Baylor College of Medicine, where he laid the foundation for his observations of abnormalities in cell structures.

In 1982 Perry joined the faculty of Case Western Reserve University, where he currently holds an adjunct appointment. He is distinguished as one of the top Alzheimer's disease (AD) researcher with over 1,000 publications, one of the top 100 most-cited scientists in neuroscience and behavior, and one of the top 25 scientists in free radical research. Perry has been cited over 77,000 times (H=140) and is recognized as an ISI highly cited researcher.

Perry is editor for numerous journals and is editor-in-chief for the Journal of Alzheimer's Disease, the most cited and prolific journal in his field. He is a fellow of the American Association for the Advancement of Sciences, Microscopy Society of America, International Engineering and Technology Institute, Texas Academy of Sciences, Association of Biotechnology and Pharmacy (FABAP), Royal Society of Chemistry (FRSC, CChem), Royal Society of Medicine, Royal College of Pathologists (FRCPath), Royal Society for the encouragement of Arts, Manufacturers and Commerce (FRSA), Royal Society of Biology (FRSB, CBio,

CSci, CSciTeach), Linnean Society of London (FLS), Royal Microscopical Society (FRMS), World Academy of Medical Sciences (FWAMS), and EU Academy of Sciences. He is past-president of the American Association of Neuropathologists and the Southwestern and Rocky Mountain Division of the American Association for the Advancement of Science, and a Foreign Correspondent Member of the Spanish Royal Academy of Sciences, Foreign Corresponding Member of the Academy of Sciences of Lisbon, Corresponding member of the Mexican Academy of Sciences, Doctorado Honoris Causa (Hon. D.)-Universidad Arturo Prat, Iquique, Chile, and member of the Iberoamerican Molecular Biology Organization. He won the Distinguished Professional Mentor award from the Society for the Advancement of Chicanos and Native Americans in Sciences, Senior Investigator Award-International College of Geriatric Psychoneuropharmacology, Martin Goland Award- Alamo Chapter Sigma Xi, UDAAN-Lifetime Achievement Award, Top Specialist in Alzheimer disease- Expertscape, Albert Nelson Marquis Lifetime Achievement Award- Marquis Who's Who, International Engineering and Technology Institute-Annual Scientific Award 2017, Denham Harman Award-American Aging Association, Zenith Award and Temple Award-Alzheimer Association, Mensch Award-Alzheimer Research Forum, Notaveis dos Azores, Scientist of the Year-Portuguese Tribune, Senior Fulbright Fellow and the Panama National Plaque of Honor for Excellence in Neuroscience.

Perry's research is primarily focused on how Alzheimer disease develops and the physiological consequences of the disease at a cellular level. Over the past 35 years, he has dissected just about every aspect of the cytopathology of AD, including the role of neurons and glia in plaque formation, cytoskeletal transformation to form abnormal filaments of neurofibrillary tangles and neuropil threads, and vascular atrophy during the course of AD. He is probably best known for his studies of oxidative modification, redox metal homeostasis, stress response, and mitochondrial dynamics. Nearly 20 years ago, based on these studies, Perry proposed that amyloidβ has antioxidant activity related to its binding of copper, and

that amyloidβ is a protective response to metabolic failure of AD. This proposal predicted the decades-long failure of therapy focused on amyloidβ removal. Perry's proposal is supported by recent work showing diet and lifestyle, both metabolic modifiers, can greatly reduce the risk of AD. Currently he is using imaging mass spectroscopy and advanced electron microscopy to analyze the atomic structure of the pathology and involvement of ferroptosis in neuronal cell death. These studies are providing the foundation for ongoing clinical trials of compounds that modulate metabolism, stress response, and metal homeostasis.

New Aspects of Experimental Physics of Interfaces

by Hans-Jürgen Butt, Member EUAS

Short Biography

1986 Diploma in Physics from the University of Hamburg, Germany
1989 PhD in Biophysics with the thesis "Time-resolved measurement of proton translocation by Bacteriorhodopsin supervised by Ernst Bamberg, Max Planck Institute of Biophysics, Frankfurt, Germany
1989-1990 Postdoc, Group of Prof. Dr. P.K. Hansma, University of California, Santa Barbara: Atomic force microscopy
1990-1996 Group of Prof. Dr. E. Bamberg, Max Planck Institute of Biophysics, Frankfurt
1995 Habilitation in Biophysical Chemistry at the University Frankfurt on Atomic force microscopy of biological objects
1996-2000 Associate Professor of Physical Chemistry at the University Mainz, Germany
2000–2002 Full-Professor of Physical Chemistry at the University of Siegen
2002 Director at the Max Planck Institute for Polymer Research Mainz

Appointments

2004 Honory Professor at the University Mainz
2007-2008 Member Fachkollegium German Research Society (DFG) for physical chemistry of molecules, liquids, interfaces, theoretical chemistry
2007-2011 Member steering committee graduate school of Excellence "Materials Science in Mainz"
2007-2014 Member steering committee center of Excellence "Smart Interfaces" in Darmstadt
2007-2011 Chair of the German Colloid Society
2008-2014 Spokesperson International Max Planck Research School for Polymer Materials
2009 Council member International Association of Colloid and Interface Scientists (IACIS)
2009 Honory Professor at the Technical University Darmstadt
2010-2016 Treasurer of the European Colloid and Interface Society (ECIS)
2015 President-Elect International Association of Colloid and Interface Scientists (IACIS)
2016 Member Fachkollegium of the German Research Society (DFG) for Polymer Research
2016 Senior member of the Gutenberg Academy of the University of Mainz

Prices and Honors

1996 Heisenberg fellowship
2008 Tewkesbury Lecture in Melbourne, Australia
2008 ICI distinguished Lecturer, University of Edmonton, Alberta, Canada
2011 Lectureship Award, Division of Colloid & Surface Chemistry, Chemical Society of Japan
2013 ERC Advanced grant: Superamphiphobic Surfaces for Chemical Processing
2017 Member of EU Academy of Sciences

Overview

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

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

Super Liquid Repellency

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

1. Using confocal microscopy we image water drops advancing on a superhydrophobic array of micropillars. In contrast to common belief, advancing and receding are fundamentally different processes. When advancing, the liquid surface gradually bends down until it touches the top face of the next micropillars. On the receding side, pinning to the top faces of the micropillars determines the apparent receding contact angle. Receding contact angle should be used for characterizing superliquid repellent surfaces rather than the advancing contact angle (Schellenberger et al., *Phys. Rev. Lett.* **2016,** *116*, 6101. Highlighted by *Nature Materials* **2016**, *15*, 376).

2. **Enhancing CO_2 capture using robust super amphiphobic membranes**. Gas membranes are used to exchange gas between the gaseous and the dissolved phase in a liquid. They are essential for many processes in chemical engineering. We aim to fabricate and test superamphiphobic gas membranes. The hope is that such membranes are more efficient than conventional gas membranes and that they reduce clocking and biofilm formation. As one important example we introduce superamphiphobic membranes for enhanced CO_2 absorption (Geyer et al., *Adv. Mater.* **2017**, *29*, 1603524.). The CO_2 capture rates of our membranes were enhanced by more than 20%.

3. **Beyond the Lotus effect: Self-cleaning photocatalytically active PDMS-coated-TiO_2**. Many superhydrophobic surfaces show a self-cleaning effect. Dust particles, adhering to the surface, are washed off by water drops. This self-cleaning effect keeps many biological surfaces such as leaves of the lotus plants free of dust. For artificial surfaces contamination by oily substances, however, limits the duration of the effect. One step towards self-cleaning also of organic contamination is to use metal-oxide photocatalysts (MOPCs) such as TiO_2, ZnO, SnO_2, CeO_2, Ag_2O, Fe_2O_3, WO_3, and

V_2O_5. They create reactive free radicals by generating electron-hole pairs under light irradiation. This photocatalytic activity causes oxidation or decomposition of most organic molecules and leads to several secondary reactions. We demonstrate how MOPCs can be coated in a simple way with a stable brush of polydimethylsiloxane (PDMS) (Wooh et al., *Adv. Materials* **2017**, *29*, 1604637). The hydrophobic surfaces remain photocatalytic active. Superhydrophobic wetting properties are realized by grafting PDMS on hierarchical-structured MOPCs. Therefore, the superhydrophobic PDMS-MOPC surfaces combine self-cleaning properties with chemical degradation of contaminants. PDMS-coated MOPC nanoparticles can also be dispersed in non-polar organic solvents. Furthermore, to create photocatalytically active lubricant impregnated surfaces we infused mesoporous PDMS-coated-TiO_2 with silicone oil (Wooh & Butt, *Angew. Chemie Intl. Ed.* **2017**, *56*, 4965). Liquid drops such as water, methanol and even low surface tension fluorocarbons, slide on the surface with tilt angles below 1°.

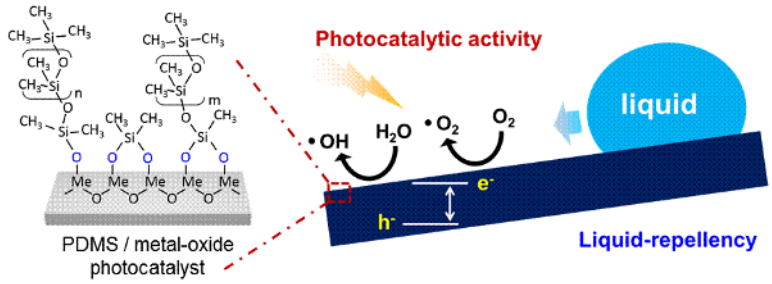


Figure 1. Hydrophobic metal-oxide photocatalysts (MOPCs) are fabricated via polydimethyl-siloxane (PDMS) grafting reaction. The PDMS brush grafted MOPCs displays omniphobic and superhydrophobic properties on flat and hierarchical structure, respectively, while keeping its photocatalytic activity that realizes effective self-cleaning and anti-biofouling surfaces.

Dynamics of Wetting

It has been known for more than 200 years that the maximum static friction force between two solid surfaces is usually greater than the kinetic friction force. In contrast to solid–solid friction, there is a lack of understanding of liquid–solid friction, i.e. the forces that impede the lateral motion of a drop of liquid on a solid surface. We found that the lateral adhesion force between a liquid drop and a solid can be divided into a static and a kinetic regime (Gao et al., *Nature Physics* **2017,** DOI: 10.1038/NPHYS4305). This striking analogy with solid–solid friction is a generic phenomenon that holds for liquids of different polarities and surface tensions on smooth, rough and structured surfaces.

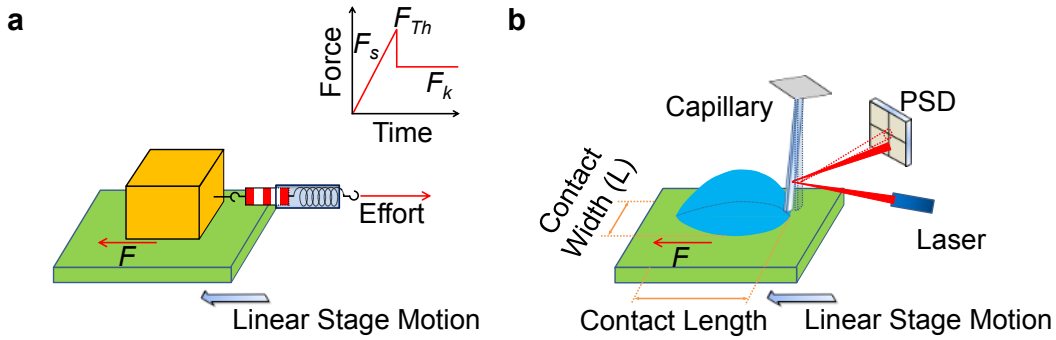


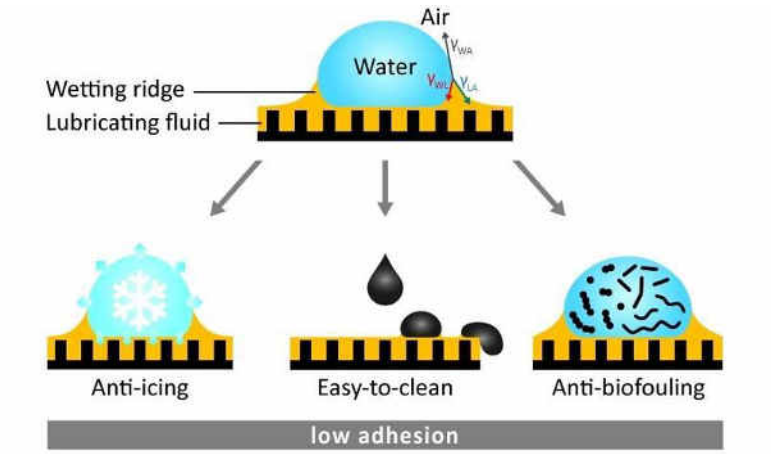
Figure 2. Schematics of friction force measurements. a, Textbook configuration for demonstrating solid–solid friction. b, Homemade setup for measuring liquid–solid friction. A drop of liquid is placed on a solid substrate mounted on a linear stage driven by a step motor. A laser beam incident on the capillary is reflected to a position-sensitive detector (PSD). The contact width between the drop of liquid and the solid surface (orthogonal to the direction of motion) and contact length (parallel to the direction of motion) are simultaneously monitored by cameras (not shown).

Surface Forces

With respect to surface forces we analyzed the interaction between soft surfaces. Micro- and nanoscale indentation is the primary approach to characterize local mechanical and interfacial properties on small scales. For soft or biological materials, quantifying mechanical properties is difficult because surface tension and surface stress play a critical role. We combine the colloidal probe technique and confocal microscopy to experimentally characterize the force indentation and force-contact radius relationships during microindentation of soft silicones (Pham et al., *Phys. Rev. Materials* **2017**, *1*, 015602). We demonstrate that the widespread Johnson-Kendall-Roberts theory must be extended to predict the mechanical contact for such soft materials. With a simple analytical model, we illustrate that accounting for the contribution of liquid surface tension, in addition to solid surface stress, helps describe the mechanical contact behavior.

ITN: Lubricant Impregnated Slippery Surfaces

In 2017 one of the coworkers in the group, Dr. Doris Vollmer, together with 15 colleagues successfully applied for an ITN. The topic is lubricant impregnated slippery surfaces (LubISS). The LubISS project aims to explore the expansive potential of lubricant impregnated surfaces, focusing on three applications of high societal, environmental, industrial and medical impact: Anti-icing, easy-to-clean and anti-fouling. Characteristic for lubricant impregnated slippery surfaces (LubISS) is that the textured or porous surface is impregnated by a liquid or a gel. The mobility of the lubricating film greatly reduces the (lateral) adhesion. Deposited liquid or solid particles, bacteria or other microorganisms can slide off easily as soon as the surface is tilted by a few degrees. However, LubISS face the problem of limited durability, the lubricant needs to be replenished after some time. To develop durable and environmentally friendly LubISS, the understanding of the interplay, and the physical- and chemical interactions between the solid surface topography, the lubricating film and the liquid (liquid and solid particles, bacteria, etc.) under static and flow conditions is necessary. The LubISS network aims to provide this understanding and will make use of it to design durable LubISS. Their performance will be tested under indoor and outdoor conditions.



Quantum Dot Based Photonics: The Markets are now coming

by Dieter H. Bimberg, Member EUAS

Short Biography

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

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

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

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

His research interests include the growth and physics of nanostructures and nanophotonic devices, ultrahigh speed and energy efficient photonic devices for future datacom systems, single/entangled photon emitters for quantum cryptography and ultimate nanomemories based on quantum dots.

Abstract:

Semiconductor Quantum Dots show a wealth of advantages as gain material for photonic (and probably electronic) devices leading to much more energy efficient and temperature stable photonic systems with applications ranging from the automotive sector to access networks. How did this (r)evolution start and where do we stand? It's a story of errors and recent brake-throughs.

The advent of semiconductor nanostructure based photonics occurred more than 40 years ago. 1976 Ray Dingle and Chuck Henry from Bell Labs received a US patent entitled "Quantum effects in heterostructure lasers" [1]. The essential argument of the patent was, that a "reduction of dimensionality", going from three dimensional material, double heterostructure (DH) lasers, to two dimensional materials, quantum well lasers, and eventually to one dimensional materials, quantum wire lasers, leads step by step to an order of magnitude reduction of the threshold current density of the lasers. Almost all semiconductor lasers in use today are indeed quantum well lasers. Their

fabrication is easy. The epitaxial growth sequence is slightly modified as compared to 3 layer DH lasers by extending it to a 5+ layer separate confinement concept, where the gain layer(s) has a thickness in the nm range (a physicist would say: below the de Broglie wavelength). For reasons of a complex, unreliable fabrication tchnology quantum wire lasers never demonstrated their theoretical advantages or made it to market. Interestingly, Dingle and Henry did not fully complete their chain of arguments by discussing potential advantages of zero dimensional structures.

It took 10 years to 1986, when a group of researchers around Suematsu at Tokyo Institute of Technology presented a detailed comparison of gain, threshold current density,… for GaAs and InP-based 0 (quantum box) to 3 dimensional lasers predicting enormous performance advantages of quantum box lasers. Earlier, in 1982, Arakawa and Sakaki had investigated QW-lasers in high magnetic fields and observed a reduction of temperature dependence of threshold current with increasing magnetic field, correctly thought to be due to increasing carrier localization. All these and other theoretical predictions were based on considering solely *lattice matched* structures. Lattice match was considered to be imperative for heterostructures at that time to avoid dislocations. Many groups in the world embarked on trying to fabricate lattice matched quantum box (today called "dot") lasers, by combining lithography with epitaxy. Seven years later such a laser based on the best available technology was presented, operating in a pulsed mode at 77 K showing a huge threshold current density. It was a discouraging disaster, however not disproving the qualitative predictions of theory.

A new dawn appeared in 1993/4, when self-organization at semiconductor surfaces upon deposition of a few *monolayers of non-lattice matched* material was discovered to lead to the formation of coherent (meaning defect-free) self-similar nm-sized pyramids, quantum dots [2], see Fig. 1 . The fabrication of such *self-organized* QDs, similar to that of QWs, is based on a non-disruptive technology, which can be adapted to any strained material system (e.g. InN/GaN). It relies simply on modifications of classical semiconductor epitaxial processes (let it be MBE or MOCVD), and uses a before undiscovered parameter window for the growth of *defect-free strained layers*, see Fig. 1. Complex and costly electron beam lithography is not used. The electronic and optical properties of such QDs, like the wavelength of radiative recombination, turned out to be size and shape dependent.

We are used since ever to manipulate the properties of materials by changing its composition. In the nanoworld we can use variations at purpose just of the geometry, without changing the composition, as a new tool for designing material properties. One of the first important subsequent discoveries was the observation of efficient recombination at 1.3 µm of InAs QDs inserted in GaAs, a wavelength typically only accessible by the InP material system. The material gain of InAs QDs turned out to be orders of magnitude larger than that of the same 3D material. QD dot layers could be easily stacked many times such that their modal gain is as large or larger than that of stacked QWs.

"Self-similarity" of QDs does not mean identity. Adjacent QDs do not contain 100% identical number of atoms, or identical interfaces, but have similar shapes, thus symmetry properties. Such identity is (fortunately for almost all device applications) prevented by entropy. The density of states of a single QD is described by a delta-function, similarly its emission line shape (see Fig. 2), which additionally shows a temperature dependent Lorentzian broadening. Thus the spontaneous emission of let's say the active area of a 100 µm wide and 1 mm long edge emitting laser, containing 10 exp 11 non-interacting QDs/cm2 is composed of the emission of 10 exp 8 QDs, each emitting at a very slightly different wavelength. Their superposition leads to a Gaussian shaped envelope typically having a half width of 30-100 meV, depending on growth conditions. The ability of generating fs pulses by mode-locked QD-lasers, or ultra-fast multiple wavelength amplification without cross-talk by semiconductor optical amplifiers results from this Gaussian broadening.

Insertion of stacked QD layers as gain material in lasers rapidly lead to the discovery of device properties being much superior to those of QW-based lasers [3], more superior than predicted, an observation that is not made frequently in device development.

Fig. 3 summarizes the history of threshold current densities for edge emitting lasers (EELs) in the last 50+ years. World record values below 10 A/cm2 x QD layer for QD-lasers were reported for

the first time in 2001. By developing so-called QD in QW structures and appropriate schemes of p-type doping, temperature independence of the threshold current density was achieved up to temperatures 60-70 °C. Gain of the quantum dots and index of refraction of the light guiding layer are completely decoupled, since the total number of carriers residing in the QDs is many orders of magnitude smaller than the number of carriers residing in the carrier reservoir. From there the carriers are scattered down to the QDs via Auger effect at a time scale below ps, leading to ultra-fast gain recovery upon gain depletion. Gain and phase modulation or both together are independently possible, enabling higher order modulation schemes, allowing to reach bit rates of 100 GHz and beyond. Other advantages reported [5] are:

- Suppression of filamentation for the transverse ground mode of EELs, leading to increased coupling efficiency into fibers
- Strongly improved radiation hardness and lower facet overheating, increasing the COMD level
- Stability enhancement by more than 20 dB for external optical feedback, e.g. by back reflection from optical fibers. Thus optical isolators in fiber-based systems can be frequently eliminated.

The fundamental advantages of QD-based photonic devices known since more than a decade, and billions of GaN-based LEDs and lasers based on QDs were sold and are used. The discovery of their advantages and the need for performance brake-throughs occurred in the same time window as demand, and made market penetration an easy task. Applications of GaAs- or InP-based nanodevices until very recently did not meet a pull from market. Replacement of costly long distance communication devices based on QWs by QD-based ones emitting in the 1.55 µm wavelength range was hindered by the argument "never change a winning team" and the low demand for such replacements or new installations.

Today the situation has changed. In what follows three examples of presently occurring demand and one research-like topic will be discussed: Frequency combs generated by mode-locked lasers and light amplification without O-E-O conversion for optical communication, automotive applications and finally quantum cryptography based on polarized single photon emitters.

Fiber to the home systems as the final point of metropolitan (MAN) and access (AN) networks are presently installed in huge quantities in all industrialized countries. MAN traffic hard ware installations are forecast to grow significantly faster than long-haul traffic ones. Consequently, the number, diversity and complexity of photonic devices, presenting the physical layer of the networks operating at least partly at 1.3 µm will increase rapidly. Innovative solutions are required to control power consumption and cost of the networks. InAs/GaAs QD-based photonic modules outperform devices based on other material systems or QWs at this wavelength from any point of view. They are more energy efficient, temperature stable, much lower cost and offer properties not observed for higher dimensional devices.

Mode-locked lasers, MLLs, emitting electrical and optical pulse trains present a backbone of high bit-rate optical communication networks. MLLs are utilized as optical clocks and, in combination with modulators, as transmitters for optical time-division multiplexing (OTDM) systems. They also find applications in other fields of communications, such as multi-carrier generation and all-optical sampling. Still in THz photonics or radio-over-fiber systems, the source/transmitter architecture can be simplified by using MLLs. Passively ML lasers (PMLLs) are lowest cost, since they only incorporate an additional element in the cavity, a saturable absorber, which, as well as the gain section, is simply direct current (DC) biased. The absorber ensures a self-start of ML, without an external radio-frequency (RF) reference source. Saturable absorbers based on QDs emitting at 1.3 µm exhibit fast recovery on the order of 700 fs under large reverse bias, enabling the generation of sub-picosecond pulses at frequencies of or beyond 80 GHZ, taking advantage of the large spectral width of the QD emission [6]. The timing jitter of MLLs is a result of random fluctuations of the photon density, the gain and the effective refractive index caused by amplified spontaneous emission (ASE). Compared to QWs, QD MLLs exhibit lower levels of ASE, which directly reduces the jitter. Optical back injection of a small part of the emitted pulse train leads to further jitter reduction down to ~200 fs and enables frequency tuning of the emitted pulse train. Repetition rates up to 160 GHz are shown in Fig. 4. By means of advanced modulation

formats larger spectral efficiencies or the ability to operate the system at a lower symbol rate for a desired data rate are feasible. 160 Gbit/s data transmission based on single-polarization D(Q)PSK data transmission format was also demonstrated using a hybrid MLL module combined with modulators [6].

State-of-the-art ANs and MANs use up to 40 wavelength channels, each carrying presently a data stream of typically 10 Gb/s, increasing to 40 Gb/s in the very near future. Next-generation optical networks, such as converged MANs and reach extended ANs, will cover longer distances, and accommodate larger splitting ratios (number of customers). Optical amplifiers are essential to compensate the additional losses caused by the extended reach and larger splitting ratios. Such amplifiers have to support multiple modulation formats, multi-level intensity- and phase-coded formats, as well as multi-wavelength channel amplification with low channel crosstalk, or wavelength switching by cross-gain-modulation. Low energy consumption and low cost will be equally decisive parameters as maximum bit rate in the future, to keep not only investment down, but also end of life cost and environmental concerns. Semiconductor OAs are low-cost mass products, showing reduced power consumption, smaller footprint, ease of integration in photonic integrated circuits, and broad gain spectra. In comparison to conventional bulk or quantum-well (QW) SOAs, quantum-dot (QD) -based SOAs demonstrate a number of unique properties, i.e. much fast carrier dynamics or decoupling of gain and phase dynamics pointed out above [7]. The fast gain dynamics of QD SOAs presently has been demonstrated to enable single and multi-channel amplification of intensity-coded signals with symbol rates up to 80 GBd. Nonlinear effects have been used successfully to demonstrate single and multi-channel all-optical wavelength conversion (AOWC) of intensity-coded signals with symbol rates up to 320 GBd.

Road illumination at night and/or under heavy rain in automotive traffic using semiconductor lasers is rapidly diffusing down from high end cars to mass production cars. Presently the lasers used, based on multiple stacked QWs, emit in the 900 nm wavelength range high power pulses of a typical width of 100 ns. The emission is elliptical, showing e.g. 10° x 25° beam divergence. The optical focusing and scanning systems and temperature stabilization are complex and costly. The maximum laser output power allowed, depends on the properties of the human eye and is regulated according to safety classes. For safety class 1 upon moving to emission wavelengths between 1.2 and 1.4 µm the allowed output power is increasing by a factor of ~20. The transmission of air is maximum between 1260 and 1340 nm. Thus inexpensive and temperature stable QD lasers available between 1260 and 1310 nm are ideal sources for road illumination. They can be combined with novel laser structures showing a round far field needing no complex optics [8].

Individually addressable quantum dots are a particularly active field of current research. The key element of ultimately secure communication, quantum communication, is a single-photon or q-bit emitter, needed for data encryption. Such an emitter must be able to emit just a single polarized photon on demand. For bridging longer distances quantum repeaters are needed, where an emitter emits exactly one pair of entangled photons. Both tasks can be accomplished using single quantum dots. Devices with individually addressed single QDs present deterministic integrated light sources providing non-classical emission characteristics, enabling secure bit-pattern transmission. Major steps in the realization of such a deterministic light source have recently been accomplished, such as *pin* diode structures with a spatially localized QDs and spatial filtering using a metal aperture. A breakthrough was the demonstration of selective electrical injection into a single QD. Individual addressing of just a single dot is achieved by confining the current path in a *pin* diode structure to the location of a single dot as illustrated in Fig. 4. The task was realized by using an oxide aperture with a small opening in close proximity below a dot. Q-bit repetition rates up to 1 GHz were demonstrated [9]. The success story of nanostructured photonic devices based on compound semiconductors just started. Lets look at the markets now.

I am indebted to Dr. S. Rodt for his help with the figures

Further Reading: die Referenzen werden noch zu den Originalen geändert

[1] For a review on the history of semiconductor lasers see: D.Bimberg, IEEE Photonics Society News 27, 4 (2013)

[2] V.A.Shchukin and D.Bimberg, Rev. Mod. Phys. 71, 1125 (1999)

[3] For an early review on QD-lasers see: D.Bimberg et al. IEEE J Select. Topics in Quant. Electr. 3, 196

(1997)
[4] For more recent review on QDs and QD photonics see: the chapter by D.Bimberg in "Optical Fiber Telecommunications" ed. by I.P.Kaminov, T.Li and A.E.Willner, Elsevier (2008) and D.Bimberg and U.W. Pohl, Materials Today 14, 388 (2011)
[5] For more details see D. Bimberg, El. Letters 44,168 (2008)
[6] D. Arsenijevic and D. Bimberg in "Green Photonics and Electronics", G. Eisenstein and D. Bimberg eds., Springer Verlag, Cham 2017
[7] H. Schmeckebier and D. Bimberg in "Green Photonics and Electronics", G. Eisenstein and D. Bimberg eds., Springer Verlag, Cham 2017
[8]D.Bimberg et al., Proc. SPIE 76161,1 (2010)
[9]A review is: W. Unrau and D. Bimberg, Laser and Photonics Review 8, 276 (2014)

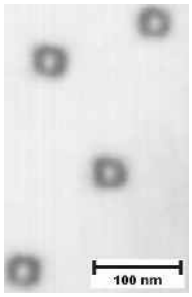


Fig. 1 High-resolution top-view transmission electron microscopy picture of a layer of InAs/GaAs quantum dots, showing four pyramidal dots. The basis of the pyramids are oriented parallel to [100] directions of the semiconductor, from Ref. 4.

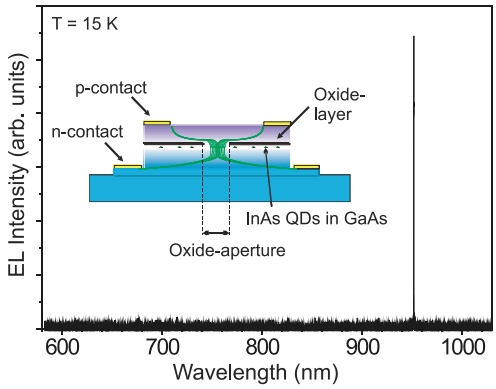


Fig. 2 Electroluminescence delta-function-like spectrum of a single quantum dot embedded in a p-i-n diode (see Fig. 6). The emission line actually consists of a superposition of two polarized emission lines a few hundred μeV apart from each other, which are not resolved in this picture. It is remarkable, that across a range of 400 nm only the emission of this single QD is observed, from Ref. 9.

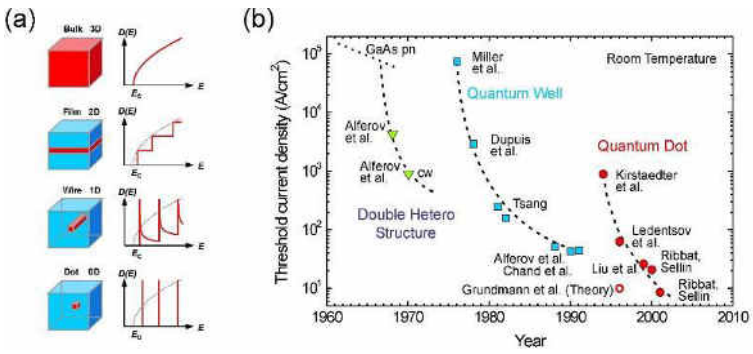


Fig. .3 Threshold current density variation of diode lasers by 4 orders of magnitude from homojunction, to heterojunction, to quantum well and finally to quantum dot based structures in the last 50+ years, from Ref. 4

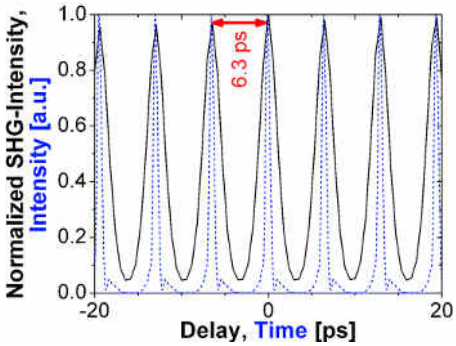


Fig. 4 Repetition rate of a chirp compensated QD MLL pulse comb at 160 GHz using an optical time division multiplexer, SHG autocorrelation measurement (black) and corresponding pulse comb (blue), from Ref. 4

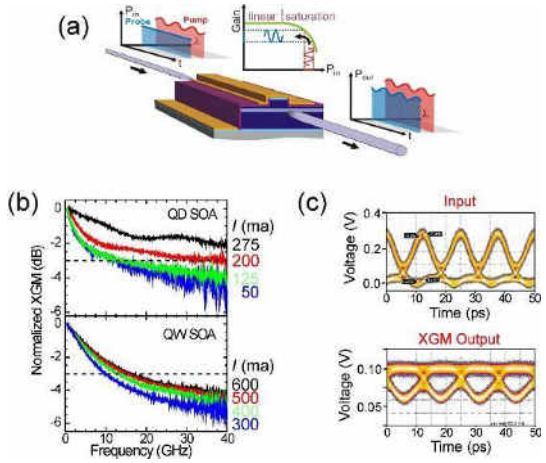


Fig. 5 Cross-gain modulation of a semiconductor optical amplifier (SOA). (a) Operation principle: a strong, modulated pump signal (P_{in}, red) drives the SOA into the saturation regime. Consequently, the SOA gain is also modulated. The modulation pattern can be transferred to a weak CW probe pulse at another wavelength (P_{in}, blue), yielding an inverted modulation pattern on the probe signal in the output (P_{out}, blue). (b) Efficiency of the cross-gain modulation of a QD SOA (top) and a conventional QW SOA (bottom). The 3dB bandwidth of the QD SOA marked by the horizontal line can be tuned to beyond 40 GHz at high injection current. (c) Wavelength upconversion using cross-gain modulation of a QD SOA and a pseudorandom RZ-OOK- modulation. Top: input eye diagram of a 80 Gb/s signal at 1292 nm wavelength, bottom: upconverted output signal at 1300 nm.

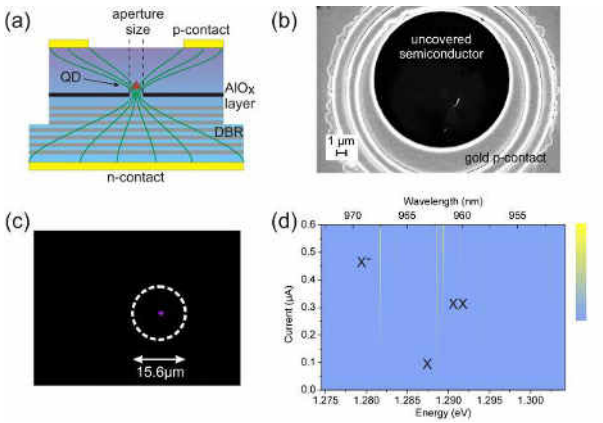


Fig. 6 Schematic cross section of a single electrically driven q-bit emitter showing the QD-position, aperture size and current flow, from Ref.9

Fabric Formwork: A New Form of Architecture

by Tim Ibell, Member EUAS

Short Biography
Sir Kirby Laing Professor of Civil Engineering, University of Cambridge, UK
Fellow of the Royal Academy of Engineering
President of the Institution of Structural Engineers 2015
Fulbright Distinguished Scholar Award 2002
Winner of six best journal paper awards
Head of the Department of Architecture and Civil Engineering, University of Bath, UK, 2005-2008 and 2010-2013
Associate Dean for Research in the Faculty of Engineering and Design, University of Bath, UK, 2014-2017
Author or co-author on around 200 papers
Member of the 2014 Research Excellence Framework Civil & Construction Engineering sub-panel
Chair elect of the Joint Board of Moderators for Civil Engineering in the UK

Concrete, our most widely used construction material, is a fluid that offers the opportunity to economically create structures of almost any geometry. Yet this unique fluidity is seldom capitalised on, with concrete instead being cast into rigid prismatic moulds to create high material use structures with large carbon footprints. My team's research demonstrates how replacing conventional orthogonal moulds with a flexible system comprised primarily of low cost fabric sheets can utilise the fluidity of concrete to create extraordinary possibilities for highly optimised, architecturally interesting, building forms.

The language and technology of concrete construction has changed dramatically over the past two thousand years - from the dome of the Pantheon, through its renaissance in the 1800s, and up to the work of Nervi and other modern masters of this fluid material. Throughout this, concrete has been cast almost exclusively into wooden or steel moulds to create prismatic elements. Nervi noted that:

> *'although reinforced concrete has been used for over a hundred years and with increasing interest during the last few decades few of its properties and potentialities have been fully exploited so far...the main cause of this is a trivial technicality: the need to prepare wooden forms' (Nervi, 1956)*

This triviality pervades the minds of Engineers even today, with increased cost being associated with concrete structures that deviate from the use of flat panels of timber or steel as formwork. Despite this, concrete remains one of the most widely used man-made materials in the world, with global production of cement approaching 3.4×10^9t in 2011 (USGS, 2011). Cement accounts for a large proportion of the world's raw material expenditure, reaching nearly 33% of the total in 2008 (Orr, 2012). Although concrete has a relatively low embodied energy (Hammond and Jones, 2011), its rate of consumption

means that cement manufacture alone is estimated to account for some 5% of global CO_2 emissions (Orr, 2012).

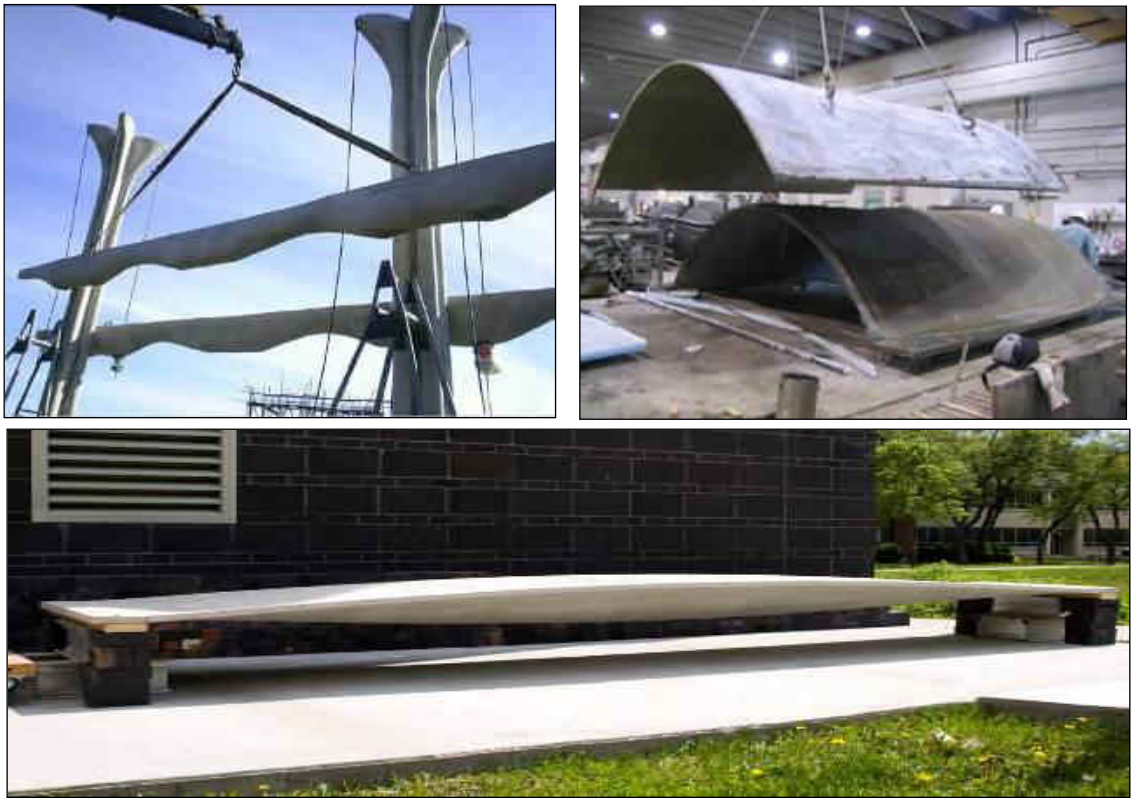


Figure 1: Possibilities using fabric formwork (Courtesy of Mark West)

Against a backdrop of carbon dioxide emission reduction targets, a recognition of the impact construction has on the environment and an increasing client focus on sustainability, design philosophies centred around the need to put material where it is required are becoming increasingly desirable. Recent research has shown that for concrete structures, large reductions in embodied carbon can be achieved simply by replacing conventional orthogonal moulds with lightweight, high strength, low cost sheets of fabric. This 'flexible formwork' not only provides environmental benefits, but also provides a new form of architecture for concrete structures as shown in Figure 1.

The architectural delight of fabric-formed concrete is an additional advantage to the material savings which can be achieved through the structural optimisation processes made possible by the use of a flexible mould. Research undertaken at the Building Research Establishment Centre for Innovative Construction Materials (BRE CICM) at the University of Bath has shown that by following simple optimisation routines and casting concrete into a flexible mould, material savings of up to 40% can be achieved in reinforced concrete beams (Garbett, 2008; Orr, 2012; Orr et al., 2011; Orr et al., 2012c).

In addition to significant material use reductions, research at the BRE CICM has demonstrated that permeable fabric formwork can provide concrete with enhanced durability when compared to concrete cast against an impermeable surface. Significant reductions in carbonation depth and chloride ingress have been recorded (Orr et al., 2012a).

From this, it is apparent that the use of fabric formwork can provide:

- Material use reductions by replacing conventional orthogonal structures with non-prismatic, structurally efficient, alternatives;
- Enhanced durability by the provision of a permeable formwork system;
- New forms of concrete architecture.

Flexible formwork therefore has the potential to facilitate the change in design and construction philosophy that will be required for a move towards a less material intensive, more sustainable, construction industry. The main feature of all concrete elements cast in flexible formwork is that their final shape is not known precisely in advance. The cross section of a fabric-formed beam is defined by the deformation of the fabric membrane under the hydrostatic pressure applied by the fresh concrete. Therefore, the cross section of the hardened concrete beam has to be predicted by an appropriate form-finding method for a set of boundary conditions dependent upon the construction approach. In general, the design of fabric-formed beams combines a form-finding procedure with structural analysis, which then can be extended to allow optimisation for defined loading envelopes and geometrical constraints.

By replacing orthogonal concrete moulds with a system formed of flexible sheets of fabric it is possible to construct optimised, variable cross section concrete elements that can provide material savings of up to 40% (Orr, 2012) when compared to an equivalent strength prismatic member.

The principle behind the design of beams using fabric formwork is that at each section along the length of the beam, the resistance of the beam (in flexure, shear, torsion and so on, R_d) matches the requirements of the design envelope (E_d). This simple principle of setting $R_d = E_d$ can create complex shapes – which can then be constructed using the flexible fabric mould. Although much structural testing has focused on beams, this optimisation process (and fabric formwork) can be used for many other structural forms (as seen in work presented in Orr et al (2012c)).

Accurate shape predictions for fabric cast concrete elements (beams, column, shells and so on) are essential. Scale models (using plaster) have been successful, and new techniques have simply replaced physical models with virtual ones. Methods used include simple spreadsheets which predict the hydrostatic shape of the fluid filled fabric (mathematically explained by Iosilevski (2010)) to more complex computer programs that can automate the entire process (Veenendaal, 2008). The form-finding approach adopted here is based on a numerical iterative procedure (Foster, 2010). The procedure can be used to find the coordinates of points equally spaced along the length of the fabric i.e. describe fully the cross sectional curve profile. Figure 2 highlights the concept of the procedure using the constant relationship between the hydrostatic height z_i at any given point of the curve and the angle between the tangents to the curve at the same point θ_i, to calculate the coordinates x_i and y_i at each iteration step.

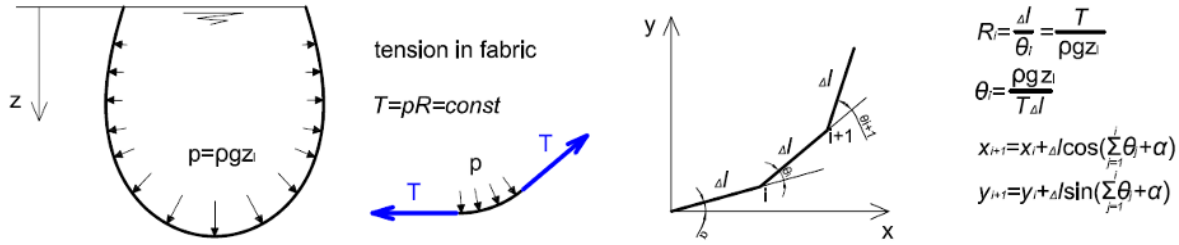


Figure 2: Form-finding procedure

In addition to the important structural advantages of fabric formwork, further possibilities are found in architecture. In teaching, fabric formwork has been successfully used at multiple Universities as a means to consider not only how Engineers and Architects undertake efficient design, but also to 're-think' how concrete itself should be used as a structural material.

References

Araya, R. and West, M. 2012. Flat sheet fabric moulds for double curvature precast concrete elements. *In:* Orr, J. J., *et al.* (eds.) *Second International Conference on Flexible Formwork* University of Bath: Bath.

Bailiss, J. 2006. *Fabric-formed Concrete Beams: Design and Analysis.* M.Eng. Dissertation, University of Bath, UK.

Foster, R., 2010. Form finding and analysis of fabric-formed concrete beams. M.Eng. Dissertation, University of Bath, UK.

Garbett, J. 2008. *Bone Growth Analogy for Optimising Flexibly Fomed Concrete Beams.* M.Eng. Dissertation, University of Bath, UK.

Hammond, G. P. and Jones, C. I. 2011. Embodied energy and carbon in construction materials. *Proceedings of the Institution of Civil Engineers: Energy,* 161 (2), 87-98.

Jelic, I. 2002. *Behaviour of Reinforced Concrete Beams: A Comparison between the CFP Method and Current Practice.* Ph.D. Thesis, Imperial College London, UK.

Kotsovos, M. D. 2007. Concepts underlying reinforced concrete design: Time for reappraisal. *ACI Structural Journal,* 104**,** 675-684.

Nervi, P. L. 1956. *Structures*, FW Dodge Corp.

Orr, J. J. 2012. *Flexible Formwork for Concrete Structures.* Ph.D. Thesis, University of Bath, UK.

Orr, J. J., Darby, A. P., Ibell, T. J. and Evernden, M. 2012a. Durability enhancements using fabric formwork. *Fib symposium: Concrete structures for Sustainable Community.* Stockholm, Sweden.

Orr, J. J., Darby, A. P., Ibell, T. J., Evernden, M. C. and Otlet, M. 2011. Concrete structures using fabric formwork. *The Structural Engineer,* 89**,** 20-26.

Orr, J. J., Darby, A. P., Ibell, T. J., Lava, P. and Debruyne, D. 2012b. The shear behaviour of non-prismatic concrete beams determined using digital image correlation (submitted for publication). *In:* Dirckx, J. (ed.) *5th International Conference on Optical Measurement Techniques for Structures and Systems 2012.* Antwerp, Belgium.

Orr, J. J., Evernden, M., Darby, A. P. and Ibell, T. J. 2012. Proceedings of the Second International Conference on Flexible Formwork, 27th-29th June 2012c Bath, UK. University of Bath.

USGS. 2011. *Minerals Information* [Online]. US DoI, USGS. Available: http://minerals.usgs.gov/minerals/ [Accessed 01/01 2013].

Veenendaal, D. 2008. *Evolutionary Optimisation of Fabric Formed Structural Elements.* Masters, University of Delft, The Netherlands.

West, M. and Araya, R. 2012. Recent fabric formwork construction projects. *In:* Orr, J. J., *et al.* (eds.) *Second International Conference on Flexible Formwork.* University of Bath: Bath.

Innovative Aspects in Tribology, Fatigue & Damage Analysis

by Michael Khonsari, Member EUAS

Short Biography

Dow Chemical Endowed Chair and Professor of Mechanical Engineering
Director, Center for Rotating Machinery - Louisiana State University

Michael Khonsari earned his B.S., M.S., and Ph.D. all in Mechanical Engineering from The University of Texas at Austin. Dr. Khonsari holds the Dow Chemical Endowed Chair in Rotating Machinery and Professor of Mechanical Engineering at Louisiana State University (LSU). Prior to joining LSU, he spent a number of years as a faculty member at The Ohio State University, University of Pittsburgh, and served as the Chairman of the Department of Mechanical Engineering and Energy Processes at Southern Illinois University. Professor Khonsari has also served as a research Faculty Fellow at NASA Glenn (formerly, Lewis) Research Center, Wright-Patterson Air Force laboratories, and the U.S. Department of Energy. In February 2003, Professor Khonsari was appointed as the Louisiana Experimental Program for Stimulating Competitive Research (EPSCoR) Project Director and Associate Commissioner for Sponsored Research & Development Programs at the Louisiana Board of Regents.

Professor Khonsari's research is in the area of tribology—the science and application of lubrication, friction, and wear—and fatigue and damage analysis. He is the holder of several US patents, has authored over 280 archival papers, 50 book chapters and special publications, three technical books and delivered over 180 invited lectures, seminars, and plenary presentations. Professor Khonsari is the recipient of several research awards including the ASME Mayo Hersey Award, Burt Newkirk Award, the STLE Presidential Award, ALCOA awards for his contributions to tribology, and is the recipient of the LSU Distinguished Research Master Award and inducted into the Academy of Distinguished Mechanical Engineers at University of Texas at Austin. Professor Khonsari is the Editor-in-Chief for ASME Journal of Tribology and serves on the Editorial Board of STLE Tribology Transactions, Institution of Mechanical Engineers Journal of Engineering Tribology, Tribology International, Advances in Tribology, and Patents on Mechanical Engineering, Lubricants, and Entropy. Professor Khonsari is a fellow of American Society of Mechanical Engineers (ASME), Society of Tribologist and Lubrication Engineers (STLE), and American Association for the Advancement of Science (AAAS).

Research and Development

Professor Khonsari is the founding Director of the Center for Rotating Machinery (CeRoM) at LSU. CeRoM is dedicated to state-of-the-art research and development associated with rotating machinery. The Center's R&D activities include the following areas: tribology addressing lubrication, friction, and wear; dynamics and vibration analysis of machinery; materials selection, fatigue and damage analysis; measurement, testing, and sensing; modeling and simulation; and education. These activities will directly support improvements in design, manufacturing, diagnostics, reliability, performance, durability, and environmental compliance of vital mechanical systems and components, including but not limited to bearings, seals, gears, turbines, compressors, and generators.

Professor Khonsari has made the "game-changing" contribution to the theory and methodology for assessment of lifetime prediction of materials and components subjected to degradation forces such as fatigue and wear. He has established the foundation of the framework for the science of degradation via thermodynamics and demonstrated its applications experimentally. Researchers around the globe are making use of these principles with remarkable success. Khonsari is world renowned and recognized as the leading authority on the tribology of mechanical components and the developer of the most comprehensive

performance prediction and bearing design tools. His thermohydrodynamic analysis of bearings, for example, has settled a controversy on the influence of lubricant supply temperature on the threshold of whirl instability that existed in the literature over 60 years. His seminal contributions to the understanding of the nature of thermoelastic instability and thermally-induced seizure of components and have developed scientific methodologies to guard against their failure. Khonsari's research has a tremendous impact on the improving the design, performance, and reliability of bearings, mechanical seals, pumps, compressors, turbines, generators, and the like.

Multidisciplinary Research and Education

Professor Khonsari has led several large multidisciplinary teams of scientists and engineers that worked collaboratively on the funded research of national innovative and scientific importance. Currently, he leads a collaborative team from several institutions to establish a $20M Consortium for Innovation in manufacturing and materials funded by NSF. He has been Principal Investigator of research grants and contracts totaling over $100M (mostly from NSF). He has directly supervised and mentored over 70 PhD, MS, and post-doctoral students and scholars. His students are highly sought after by industry and academia and hold important positions including serving as a university president. Khonsari is an avid promoter of science and engineering education. As an example, to inspire the next generation of scientists and engineers, Khonsari leads several STEM education & outreach that has engaged over 30,000 K-12 students over the past 5 years alone. Dr. Khonsari has the unique ability to reduce the complexities of material degradation to concepts that readily resonate with students and these outreach activities are at the core of exciting the young minds to become the innovators of tomorrow.

Statewide Policy and Strategic Planning for Science and Technology

Professor Khonsari is appointed by the Governor to serve on the Louisiana Innovation Council, whose mission is "mission is to establish a comprehensive economic strategy and innovation agenda that will grow the state's economy and enhance competitiveness." Khonsari help guide the development of the research agenda for Louisiana's most recent master plan for higher education, which promotes intra-and intercampus multidisciplinary research and education, and was a participant in crafting the State's Science and Technology Plan: Fostering Innovation through Research in Science and Technology. This plan calls for investments in areas of research that are aligned with specific high-growth target industries. To this end, Khonsari has had a major role in developing programs for research and development partnerships between academia and industry.

On the thermodynamics of degradation

M. D. Bryant, **M.M. Khonsari**, F.F. Ling
Proc. R. Society A(2008) **464,** 2001-2014

Abstract

The science base that underlies modeling and analysis of machine reliability has remained substantially unchanged for decades. Therefore, it is not surprising that a significant gap exists between available machinery technology and science to capture degradation dynamics for prediction of failure. Further, there is a lack of a systematic technique for the development of accelerated failure testing of machinery components. This article develops a thermodynamic characterization of degradation dynamics which employs entropy, a measure of thermodynamic disorder, as the fundamental measure of degradation; relates entropy generation to irreversible degradation, and shows that components of material degradation can be related to the production of corresponding thermodynamic entropy by the irreversible dissipative processes that characterize the degradation. A theorem that relates entropy generation to irreversible degradation, via generalized thermodynamic forces and degradation forces, is constructed. This theorem provides the basis of a structured method for formulating degradation models consistent with the laws of thermodynamics. Applications of the theorem to problems involving sliding wear and fretting wear, caused by effects of friction and associated with tribological components, are presented.

On the thermodynamic entropy of fatigue fracture

M. Naderi, M. Amiri & **M. M. Khonsari**
Proc. R. Society A(2010) **466,** 423-438

Abstract
The entropy production during fatigue process can serve as a measure of degradation. We postulate that the thermodynamic entropy of metals undergoing repeated cyclic load reaching the point of fracture is a constant, independent of geometry, load, and frequency. That is, the necessary and sufficient condition for final fracture of a metal undergoing fatigue load corresponds to a constant irreversible entropy gain. To examine validity, we present the results of an extensive set of both experimental tests and analytical predictions that involve bending, torsion, and tension-compression of Al 6061-T6 and SS 304 specimens. The concept of tallying up the entropy generation has application in determining the fatigue life of components undergoing cyclic bending, torsion, and tension-compression.

On the Anelasticity and Fatigue Fracture Entropy in High-cycle Metal Fatigue
M. Liakat, **M.M. Khonsari**
Materials & Design **82**(2015), 18-27

Abstract

The concept of thermodynamic entropy generation in a degradation process is utilized to study the high-cycle fatigue of medium carbon steel 1018. Uniaxial tension-compression fatigue tests are carried out with tubular dogbone specimens at different stress levels and loading frequencies. It is shown that a phase lag between the stress and the strain caused by the internal friction includes a considerable amount of non-damaging anelastic energy in a hysteresis loop when the amplitude of cyclic load is substantially smaller than the yield strength of the material. A methodology is proposed to determine the anelastic energy associated with metal fatigue at a stress level lower than the yield strength of a material. Finite element Simulations are carried out with a 3-D model of the specimen to determine the validity of the proposed methodology. The evolutions of the plastic strain energy and temperature are discussed and utilized to calculate the entropy accumulation. It is shown that the accumulation of entropy generation in the HCF of the material - beginning with a pristine specimen and ending at fatigue fracture - is nearly constant within the experimental and loading conditions considered. The concept of tallying entropy is useful for the prediction of the fatigue life evolution of a material undergoing cyclic loading.

Prediction of Crack Nucleation in Rough Line-Contact Fretting via Continuum Damage Mechanics Approach
A.B. Aghdam, Ali Beheshti & **M.M. Khonsari**
Tribology Letters, **53** (2014), 631–643

Abstract
The crack nucleation behavior of rough surfaces in line contact is investigated by means of a thermodynamically-based continuum damage mechanics technique. The deterministic approach is employed to investigate the effect of roughness on the surface tractions and contact stresses. In order to treat the effect of high stress gradients, a special averaging technique, proposed previously for the case of smooth surface, is adopted in this study. The predictions of the crack nucleation life are compared with relevant experimental data in

literature, and indicate the validity of the analysis.

Thermodynamic Analysis of Fatigue Failure in a Composite Laminate
M. Naderi, **M. M. Khonsari**
Mechanics of Materials, **46** (2012), 113-122

Abstract
We put forward a thermodynamic approach for analyzing fatigue failure in a composite laminate. We show that fatigue is an irreversible progression of increasing entropy that accumulates until it reaches a critical value called the fracture fatigue entropy (FFE) at the onset of failure. Extensive series of controlled fully-reversed bending fatigue tests are carried out that involve load-controlled, tension-tension, and displacement with three different stress ratios as well as constant- and variable-loading. The role of hysteresis energy in the entropy generation is investigated. FFE values are calculated based the experimental data obtained for temperature and hysteresis energy of a woven Glass/Epoxy (G10/FR4) laminate. The concept of tallying entropy accumulation and the use of FFE are useful for determining the fatigue life of composite laminates undergoing cyclic loading.

On the role of cooling on fatigue failure of a woven Glass/ Epoxy laminate
A. Kahirdeh, M. Naderi, **M. M. Khonsari**
Journal of Composite Materials, **47** (2013), 1803-1815

Abstract
The effect of the surface cooling on fatigue life of the Glass/Epoxy laminate during fully reversed bending tests is examined. Acoustic emission and thermography are used to monitor the structural integrity and the evolution of damage. Analytical studies are performed to calculate the stress within the laminate for both cases of cooled and uncooled specimens. The results show that the life of the laminate is highly dependent on temperature and that surface cooling, if done appropriately, can significantly increase the fatigue life of the laminate.

Elliptical Point Contact of Rough Surfaces: Contact Behavior and Predictive Formulas
Ali Beheshti, **M. M. Khonsari**
Journal of Applied Mechanics, **81** (2014), 111004

Abstract
Statistical micro-contact models of Greenwood-Williamson (GW) and Kogut-Etsion (KE) are employed along with the bulk deformation of the contacting solids to predict dry rough elliptical point-contact characteristics such as the pressure profile, real area of contact and contact dimensions. In addition, the contribution of the bulk deformation and the asperity deformation to the total displacement is evaluated for different surface properties and loads. The approach involves solving the micro-contact and separation formulas simultaneously Also presented are formulas that can be readily used for the prediction of the maximum contact pressure, contact dimensions, contact compliance, real area of contact and pressure distribution.

Advanced Technologies & Diagnostic Spin-Outs

by Carl Borrebaeck, Member EUAS

Short Biography

1. Personalia
Full name: Carl A.K. Borrebaeck
Address Department of Immunotechnology, Medicon Village bldg. 406, 223 81 Lund
1. Undergraduate Studies Lund University (LU), Sweden. B.Sc. Chemistry/Math. 1974
M.Sci. Chem Eng. 1976
2. Graduate Studies Lund University, Sweden D.Sc in Mol Immunol 1979
3. Post-doctoral studies University of California, Davis, CA, USA 1980/81
4. Assoc. Prof (Docent) Lund University 1981
5. Current position Professor 1990-
Director, CREATE Health Translational Cancer Center 2006-
6. Previous positions Vice President of Lund University 2009-2014
Director of Microarray Resource Center – MARC 2005-2015
Chairman of the Wallenberg Laboratory, LU 1998-2001
Assoc. Professor of Immunotechnology, LU 1985-1989
7. Sabbatical period Distinguished Visiting Professor at OMRF
Oklahoma Medical Research Foundations, Oklahoma City 1996-1997
2. Awards
2017 The Biotech Builders Awarded 2017 for outstanding entrepreneurship
2012 Nominated and awarded the Academy of Eng. Science Gold Medal for outstanding research
2012 Nominated and awarded Research!Sweden Award for Translational Medical Research
2009 Nominated and awarded Akzo Nobel Science Award
2004 SSF - Senior Individual Grant for distinguished scientists
1996 Nominated and selected as OMRF Esther Z. Greenberg Scholar, Medical Research Foundation, Oklahoma City, USA.
3. Commissions of Trust
2017- Founding Mentor of NOME (www.nome.nu)
2009-2012 International Board Member of Cancéropôle Grand Sud-Ouest, France (French Government National Cancer Plan)
2009- Member of the Royal Fysiographic Academy (estbl. 1772)
2009-2011 Member of the Executive Board of the Faculty of Engineering (LTH)
2006 Faculty Promotor at the Professor Installation Ceremony at Lund University
2003- Royal Academy of Engineering Sciences (permanent member)
2000-2005 Scientific Advisory to the Academy of Finland
1999-2000 Chairman Biotechnol. Section, The Swedish Research Council (TFR) Executive Board
1996-2000 The Swedish Research Council for Engineering Sciences (TFR)
4. Academic Merits
1988-2016 Supervised and co-supervised >50 graduate students
1977-2016 >350 publications (h factor 45) and reviews in peer reviewed international journals.
1983-2016 Invited speaker/Key note speaker to >250 national/international meetings
5. Entrepreneurial experience

Started five biotech companies: BioInvent International AB, Stockholm Stock Exchange (SmallCap). Alligator Bioscience AB, founded 2000 (Nasdaq MidCap). Immunovia AB, founded 2007 (Nasdaq 2017-04-12
First North). SenzaGen AB, founded 2010 (Nasdaq First North). Atlas Therapeutics AB, founded 2011.
6. Experience of Infrastructures
I have been heading several large infrastructures, e.g. Swegene Genomic & Proteomic Center (2006-2015), where we annually serve >500 scientists. Co-supervised 5 large EU Consortia. Headed large Strategic research centers, such as CREATE Health (2006-) comprised of >80 members with a center support of >m$25.
7. Industrial & Financial experience:
7.1. Company Boards:
2010- Chairman of the Board, SenzaGen AB
2007- Chairman of the Board, Immunovia AB
2010- Board Member Clinical LaserThermia System AB
2010-2016 Board Member, WntRes AB
2009-2014 Chairman of Lund University Innovation System AB, Lund, Sweden
2001- Cofounder and Board Member of Alligator Bioscience AB, Lund, Sweden
1983-2013 Cofounder and Board Member of BioInvent International AB, Lund, Sweden.
1998-2007 Board Member Teknikbrostiftelsen (Technology Transfer Foundation)
2006-2010 Chairman of the Board, InnovationBridge South AB
2000 -2003 Board Member TeknoSeed AB (Seed Capital Investments)
1996-2000 Board member of Innovation Stipend Selection Committee (Teknikbrostiftelsen)
1998-2006 Chairman of the Board, Lund University Technology Transfer Group AB
1998-2000 Board Member Teknopol AB (Lund University Business Consulting)
1992-1993 Board member Pronova Oncology (Oslo, Norway)
7.2. Operative Industrial Positions
1987-2008 Senior Vice President - CSO, BioInvent Int. AB.
1990-1994 President & CEO, BioInvent Int. AB.
7.3. Financial and Capital Market experience:
1998-2010 Advisory Board Member to InnovationsKapital AB (Venture Capital)
2001-2003 Advisory Board Member to Industrifonden (Industrial Foundation - Venture Capital)
1988-1995 Research consultant to major/intermediate pharmaceutical companies in USA and Sweden

Interview with Professor Carl Borrebaeck DSc by Claire Raison (Commissioning Editor of Expert Review of Molecular Diagnostics)

What area of your work do you find most rewarding?

Most of my professional life I have been involved in and focused on biological therapy of cancer, using antibodies. Over the last decade advanced diagnostics has attracted a lot of my attention for two reasons, firstly the lead time to developed information-rich diagnostic principles is short as compared to pharma development, and secondly is the fact that a statement supported by the WHO and other bodies. The reward is to be able to bring some of these research results to society, where it will benefit patients.

What is your proudest achievement in your career so far?

Being able to take several human recombinant antibodies to the clinic: the most recent of which is an agonistic antibody against CD40, which in immuno-oncology applications has shown absolutely remarkable preclinical results against solid tumors. It was spun out into Alligator Bioscience AB (Lund, Sweden), a company I started some years ago, and was recently the basis in a very large licensing deal to Johnson & Johnson (New Brunswick, NJ, USA). Furthermore, multiparametric diagnostics for the early detection of,

for example pancreatic cancer, has been a very successful program, which has resulted in a test platformthat will be able to deliver very important data in the early and differential diagnosis in different cancer indications.

You are a key member of CREATE Health co-operative. How has the cooperative grown since its formation?

CREATE Health was founded in 2006, where our application was ranked number 1 of 114 center applications. It was formed by seven different principal investigators with expertise ranging from clinical oncology to proteomics, genomics and nanotechnology. Together with these principal investigators and my research coordinator, we have since been very successful in raising governmental funds, achieving a center financing of over US$20 million. The idea behind CREATE Health [1] was to identify unmet clinical needs and to solve these in our laboratories: in other words, to always start with a clinically defined hurdle. CREATE is an acronym for 'Cancer Research using Emerging Advanced Technologies', where several of the most advanced technologies have been developed in-house. One of the emerging and growing programs in CREATE is 'MAD for Cancer'[2], having its own steering committee and encompassing four of the major faculties at the university, including for the first time Social Sciences, where the interplay between body and mind is studied using bimolecular technologies. The CREATE Health co-operative has also grown far outside the Swedish boundaries, including collaborations with Rogosin Institute (New York, NY, USA), Tianjin Medical University Cancer Institute and Hospital (Tianjin, China), Oxford University (Oxford, UK) and the Spanish National Cancer Research Centre (CNIO) (Madrid, Spain) to mention just a few. In brief, it has been a very successful venture as judged by several international evaluations.

You have spent much of your academic career based at Lund University. Having been at the institution for so long, do you feel a particular affinity with the University? Has this shaped your career?

Lund University has been a continuous source of support, which together with time spent in the US, for example at the University of California, Davis (Davis, CA, USA) and Oklahoma Medical Research Foundation (Oklahoma City, OK, USA), has given me the scientific inspiration to develop some of the larger programs. Furthermore, being head of the Department of Immunotechnology and, for the last 6 years, Vice President of Lund University, responsible for its innovation strategies, has given me the opportunities and freedom to initiate anything from CREATE Health to Medicon Village Cancer Center (Lund). In that sense it has shaped but also allowed me to shape my career.

Has your involvement in co-founding biotech companies affected your approach to other, more academic aspects of your work?

I have been interested in the interphase between academia and industrial application for decades. I believe very strongly that it is our obligation as scientists to transfer our knowledge to the society for the benefit of its inhabitants. Furthermore, I know from experience that there is no contradiction between this attitude and the possibility of performing successful basic science. This has allowed me to co-found five companies, of which the more recent are Alligator Bioscience, Immunovia (Lund) and SenzaGen (Lund). Having participated in the processes to establish, fund and develop business strategies also

helped me to develop a very valuable skill in communicating complex scientific questions, for the benefit of attracting funding for more basic scientific programs. In summary, the symbiosis between science and commercial development has been very exciting and valuable for my academic career.

In your opinion, what are the most important unmet needs that molecular diagnostics should address?

There is no doubt whatsoever that the major challenge molecular diagnostics is facing is the ability to collect enough data to be able to deliver solutions to unmet clinical needs, such as early diagnosis, patient stratification and therapy selection. To be able to deliver this kind of evidence based data we need to expand our views and realize that multiparametric diagnostics is the solution. Multiparametric diagnostics implies that we analyze many data points – hundreds or thousands of genes or proteins – and correlate these to the clinical question at hand. Consequently, this molecular diagnostic approach would deliver massive amounts of information and truly decipher the wealth of information found in, for example, a blood sample.

What do you think are the current failings or shortcomings of molecular diagnostics? How might these be addressed?

Molecular diagnostics has during recent years started a transformation from traditional approaches to solve a problem to more advanced approaches, based on recent technology developments in affinity proteomics, next gen sequencing, mass spectroscopy and so on. This clearly demonstrates that we need to continuously focus on advanced technology development, which should go hand-in-hand with clinical applications. Why? Physicians can only manage what we can measure.

References

1. CREATE Health www.createhealth.lth.se
2. MAD for Cancer www.madforcancer.lu.se

Process Machinery & Systems Engineering

by Eberhard Schlücker, Member EUAS

Short Biography
Prof. Dr.-Ing. Eberhard Schlücker
Chair of Institute of Process Machinery and Systems Engineering
Department of Chemical and Bioengineering
Cauerstraße 4, 91058 Erlangen / Germany

Research career

Since 4/2000 Full professor and head of the Institute of Process Machinery and Systems Engineering, University of Erlangen-Nuremberg
1997-2000 Authorized signatory, LEWA GmbH, Leonberg
1997 3-month research stay, USA
1995-1997 Head of Department R&D, LEWA, Leonberg
1989-1995 Research Assistant at the Institute for Process Technology and Machinery, University of Erlangen-Nuremberg, advisor Prof. Dr.-Ing. G. Vetter
1993 Ph.D. thesis: Optimisation of circular plastomer membranes for oscillating displacement pumps
1989 Dipl.-Ing. degree in Chemical Engineering, University Erlangen-Nuremberg
1978 - 1984 Engineer for research, design and development, deputy chief of research at company Lewa, Leonberg
1978 Ing. grad. Mechanical Engineering, Technical College Heilbronn
1974 Qualification as skilled worker in machinery

Research area / activities

Eberhard Schlücker has a wide spectrum of research interests ranging from fluid-systemdynamics and fluid acoustics to chemical and biological process technology with a main focus on pumps, compressors, high pressure and process technology. E. Schlücker holds more than 250 publications, 12 patents and is leading a group of currently 40 doctoral students.

Major activities

- *Head of research project "Bavarian Hydrogen Center"*
- *Chairman of research groups (Twin-Jet, Heart Actor, DFG Research Groups)*
- *Chairman of the research group for Ammonothermal Synthesis (DFG Proposal)*
- *Founder and coordinator of the master study program "International Project Management in Systems Engineering"*
- *Chairman of the EFCE Working Party for High Pressure Technology*
- *Member of three boards in ProcessNet (German working group for plant engineering,*
- *German working group for engineering education, German working group for high pressure processes)*
- *Member of the VDMA programme committee for the Rotating Equipment-Conference*
- *VDI Bavaria, head of section for Process Technology*
- *Member of the Advisory-Board of the Pump-User-Symposium at A+M University, Houston,Texas, USA*
- *Technical Industry consulting, several companies.*
- *Editor and reviewer for various journals (Industriepumpen und Kompressoren, Pumpen und Kompressoren, CET, etc.)*
- *Guest lecturer at various European universities*

- *In charge of ERASMUS exchange program with the university of Valladolid (Spain) and the university of Turku (Finland)*
- *Cofounder of the Agrolytix company*
- *Cofounder of the Hydrogenious company.*
- *Author of several survey reports for courts.*

Research Topics of Prof. Dr. Ing. Eberhard Schlócker

The following 5 project descriptions are just a part of several research topics of Prof. Schlücker, but the most remarkable ones. Further projects are dealing with machine noise, pumps, compressors and plant engineering as well as with vibrations as reasons for damages in plants.

1. Biological plant treatment without killing insects when not necessary

It is not a secret, that in many places of the world the pollinator insects are pulled-out of agriculture areas, or even killed. This is a bad situation for such areas, and if further ignored, it can also create a heavy impact to human beings but also to the nature around. I.e. in some areas in the world human beings climb up the trees with cotton bud to pollinate trees. We cannot accept such situations not any longer, otherwise the human beings are in danger.

The reason of this situation is not only caused by an ignorant attitude of the human beings active in plant treatment, but also caused by people using chemicals somehow. They use chemicals with a poisoning or basically killing effect to insects, but also to the ground water and soil microbes and soil living forms. Typical already discussed agents are Glyphosate and the Neonicodoides. An important future goal must be to avoid such chemical stuff.

The research project described here was remarkable successful. Therefore, a company (AGROLYTIX) was founded to introduce these ideas to the marked.

The basic idea is, to encapsulate special natural agents in particles made of natural material like triglycerides containing additional contents. The first example is:

a) Bacculoviruses against the apple moth: Bacculoviruses are absolutely not dangerous for human beings. These viruses where encapsulated in Triglycerides, together with some Ultraviolet light protecting material. These particles are sprayed on apple trees and develop a protection against the apple moth at least effective as traditional agents .

b) The encapsulation of hop extract or sweet wood extract works as an effective fungicide against downy mildew. Statistically it is as good as copper (traditional fungicide, but poisoning the soil). The tests in vineyards showed perfect protection.

c) Encapsulation of insecticides together with attracting agents for the favoured insects , but not attracting bees or other insects. The particles followed perfectly the goal “attract and kill” for the sherry vinegar fly (a new problem in German vinyards, based on too warm winters).

Based on these examples we learned that each plant disease could be treated with natural agents. But we learned also, that the encapsulation conservates the agent and keep

it fresh and active over several weeks. Additionally the particles stick to the leaves (leave wax) and cannot be washed away by rain. Due to this the agriculturalists have to conduct the plant treatment less often and also not after a heavy rain. This saves energy and time.

Literature

1. M. Pemsel, M. Rossmann, R. Schatz, E. Schluecker, D. Freitag, S. Schwab, A. Scheurer: Encapsulation of Cydia pomonella granuloviruses for sustainable biotechnical pest control, Chemie Ingenieur Technik. 01/2010; 82:343-348.

2. New semiconductor materials grown in Ammonothermal Sythesis Process

The Ammonthermal Process runs at about 600 – 850 °C and pressures up to 300 MPa. The goal is here to synthetize new nitride materials. This project is conducted by a group of 6 working groups and is granted by the German DFG. Prof. Schlücker is the group speaker. In connection to this project a new method was developed to monitor the process in the High-Pressure-High-Temperature-Autoclaves with optical means (UVVIS, Raman Spectroscopy). This offered a complete new insight into such autoclaves. We could learn how the chemical reaction is developed and what side or intermediate products are developed. In-between 6 years the whole group synthesised the following new materials. InN, $CaGaSiN_3$and $Zn(Si,Ge,Sn)N_2$ .Further materials are in sight.

Based on this, success a proposal for a bigger grant from DFG for altogether 18 research groups is in the final phase.

Literature

1. Kimmel AC., Hertweck B., Steigerwald T., Alt N., Schlücker E.: Corrosion Behaviour of Nickel and Cobalt Based Super Alloys in Supercritical Ammonia Containing Acidic Mineralizers NH4F or NH4Cl**.** *EMSF (Essen, 05/08/16 - 05/11/16).*

2. Baser HH., Schwieger W., Freitag D., Steigerwald T., Schlücker E.: Solubility Studies of Sodium Azide in Liquid Ammonia by in situ Ultrasonic Velocity Measurement, Chemical Engineering and Technology (2017).

3. Schimmel S., Koch M., Macher P., Kimmel AC., Steigerwald T., Alt N., Schlücker E., Wellmann P.: Solubility and dissolution kinetics of GaN in supercritical ammonia in presence of ammonoacidic and ammonobasic mineralizers, Journal of Crystal Growth 479 (2017), S. 59-66, ISSN: 0022-024.

3. Hydrogen Energy Storage for Regenerative Energy Supply

This project was financed by the Bavarian state with a grant of 15 Million EURO. The idea was born by a team with the purpose to store Hydrogen – chemically coupled - in in a Liquid Organic Hydrogen Carrier (LOHC). And when energy is needed, the Hydrogen will be taken out (the LOHC will be dehydrogenated) and turned into current with fuel cell or used as hydrogen in a combustion motor or for chemical processes. The project was successful, therefore we founded a company – Hydrogenious – with the plan to build and sell plants based on this idea.

Literature

1. Milella VO., Kölpin A., Schlücker E.: Automatization of the storing-in part of a hydrogen storage system using Liquid Organic, Hydrogen Carriers, In: Energy Technology (2017), ISSN: 2194-4288.

2. Patrick Inhetveen, Nicolas S.A. Alt; E. Schlücker: Measurement of the hydrogenation level of dibenzyltoluene in an innovative energy storage system January 2016, Vibrational Spectroscopy 83.

3. Fikrt A., Brehmer R., Milella VO., Müller K., Bösmann A., Preuster P., Alt N., Schlücker E., Wasserscheid P., Arlt W.: Dynamic power supply by hydrogen bound to a liquid organic hydrogen carrier, In: Applied Energy (2017), ISSN: 0306-2619.

4. White Edging Crack in Rolller Bearings.

White edging crack is a very costly phenomenon i.e. in wind power stations. It is a damage in the inner region of the roller bearing parts. It looks a white crack, i.e. some millimetre below the surface. And exactly this is the problem: The damage cannot be seen by naked eyes and therefore develops in a hidden area, but can destroy bearings completely.

To investigate this phenomenon a test rig was built, to generate the development of white edging cracks . This test rig kept the bearing hermetically, could reach variable and high speed and could control the lubrication flow, the current generated and the gas which developed (i.e. Hydrogen). Measurement methods used where structure born noise, conductivity, local temperature, infrared (oil with additives – did change something in the oil?), lubrication oil flow and gas analyzation.

With this test rig some remarkable results were generated, but the problem is finally still not solved!

Literature

1. Pohrer B., Zürcher M., Tremmel S., Wartzack S., Schlücker E.: Einfluss des tribochemischen Schichtaufbaus auf die Ausbildung elektrisch induzierter Wälzlagerschäden, In: Tribologie und Schmierungstechnik 63 (2016), S. 32-39.

2. M Zuercher, V Heinzler, E Schlücker, K Esmaeili, T J Harvey, W Holweger and L Wang: Early failure detection for bearings in electrical environments; Journal: The International Journal of Condition Monitoring, Volume 8 | Issue 1 | February 2018.

Developments in Wind Engineering

by Qiu-Sheng Li, Member EUAS

Short Biography

Prof. Qiu-Sheng Li is Chair Professor of Civil Engineering and Director of Architecture and Civil Engineering Research Center at City University of Hong Kong. He graduated from Shanghai Jiao-Tong University with BEng in 1984 and from Harbin Institute of Technology with MEng in 1987. He obtained his PhD and the best PhD thesis award (Professor K.H. Hunt Medal) from Faculty of Engineering at Monash University, Australia. Before joining City University of Hong Kong in 1996, Prof. Li had seven years of working experience as a research engineer at Kajima Corporation in Japan and as a consulting engineer in MEL Consultants in Australia. During this period, he was involved in numerous wind engineering and structural dynamic studies on major building and structural developments in Asia and Pacific region. His main research interests and technical expertise are in wind engineering, industrial aerodynamics, structural engineering, structural dynamics, and computational mechanics. Over the last thirty years, his research in these fields has resulted in 280 refereed international journal papers and 4 books. Most of the journals are within the top 30% ranking in their respective disciplines according to their impact factors. Prof. Qiusheng Li is one of the most cited researchers in civil engineering according to Shanghai Ranking's Global Ranking of Academic Subjects 2016 by Elsevier. Prof. Li has received several awards and honours for his outstanding research contributions including National Natural Science Foundation of Chinese Outstanding Oversea Scientist Award, 2004 and The First Class Award of the Scientific and Technological Progress from the Ministry of Education of China, 2010. He was appointed as Cheung Kong Chair Professor by the State Education Ministry of China and Li Ka Shing Foundation, Hong Kong in 2007 and National Expert of the 1000 Talent Scheme by the Ministry of Human Resources of China in 2013, respectively. In particular, Prof. Li is the recipient of the 2016 Jack E. Cermak Medal from American Society of Civil Engineers (ASCE) in recognition of "his many contributions to wind engineering that range from fundamental to applied research" and "his contributions to structural dynamics studies on major building developments in Asia and the Pacific region". Currently, he is an associate editor of Journal of Structural Engineering, ASCE and an editorial board member of twenty international journals. Prof. Li has been a principal investigator for over 65 research grants with a total funding over HK$50 million in recent years.

Major Achievements and Activities

Tropical cyclones are one of the most destructive natural disasters in the world and have caused enormous casualty and property loss over the decades. The effective

prevention and reduction of tropic cyclone-induced disasters requires extensive knowledge of tropic cyclones, so exploring the wind characteristics and structural features of tropic cyclones is extremely important. There is actually considerable uncertainty regarding the structure of tropic cyclones, particularly a lack of information on profiles for wind over land from tropical cyclones, as required for the design of high-rise structures in tropic cyclone prone regions. Prof. Qiusheng Li's research team has been carrying out long-term observational study of the atmospheric boundary layer (ABL) wind structure and characteristics over different terrains during tropic cyclones, monsoons and thunderstorms by multi-instruments in Hong Kong and mainland China. Significant amounts of datasets including those recorded during numerous tropical cyclones and valuable wind data in the eye-wall regions of tropical cyclones have been collected. Intensive analysis of the measured wind data have been performed to obtain statistical information on profiles of wind speed and the wind turbulence parameters to evaluate the applicability of theoretical and empirical models and to develop new models. The analyzed results have been presented with respect to various terrain roughness/topographical conditions and the different stages of the life cycle of tropic cyclones. Such information is very useful in clarifying the unknown aspects of tropic cyclones within the ABL and also provided valuable information to improve codes of practice and proposed profiles of wind speed and direction, spectra and gust factor for tropic cyclone, monsoon and thunderstorm winds over different types of terrain, which are of importance for the wind-resistant design of high-rise buildings not only in Hong Kong but also in other regions of the world where typhoon or hurricane winds control the design parameters.

There is a trend of constructing more super-tall buildings in many places of the world especially in Hong Kong and mainland China. This poses new challenges for structural engineers because the current design codes which were made for ordinary tall structures are not guaranteed to fully cover the design of super-tall buildings, especially in tropic cyclone prone regions. It is thus required to understand the structural behavior of super-tall buildings under strong windstorms. Prof. Qiu-sheng Li and his research team have been conducting the field measurement of the effects of wind on high-rise buildings since 1996. More than ten super-tall buildings—including Shenzhen Pin An Financial Center (600 m high), Taipei 101 Tower (508 m), Hong Kong 2 IFC (420 m), Guangzhou West Tower (432 m), Shenzhen Di Wang Tower (384 m), and Guangzhou CITIC Plaza (391 m)—have been instrumented through installation of the developed wind and structural health monitoring (WSHM) systems with eight granted patents. This field measurement program is currently the largest full-scale experiment in the world for studying the effects of wind on high-rise buildings, which was introduced on the National Geographic Channel and the Discovery Channel as applications of innovative research works. WSHM systems, including anemometers, accelerometers, GPS, pressure transducers, Fiber Bragg Grating strain and temperature sensors, seismograph, optical fiber inclinometer and so on, have been installed into the above mentioned super-tall buildings. Comprehensive investigations of the wind effects on these high-rise structures have been conducting. Monitoring the wind effects on the super-tall buildings under harsh tropic cyclone conditions by the comprehensive WSHM systems are very useful for enhancing the understanding of wind-resistant design and habitability of super-tall buildings. This long-term field study investigated the wind-induced loads and vibration characteristics and serviceability of the high-rise structures, examine and validate the adequacy of current codes of practice for the wind-resistant design of super-tall

buildings. The field study provided important validation of design procedures and assurance of acceptable behavior. For example, based on the full scale measurement study, several damping models were proposed with the suggested range of damping ratio values for the wind-resistant design of tall buildings, which provided valuable and reliable references for the structural design. In addition, the findings of the field study aided evaluation of the ability of wind tunnel tests and numerical simulation techniques to realistically predict wind effects on super-tall buildings.

Due to most of buildings' damages during windstorms happened on low-rise buildings, Prof. Li's team built and instrumented three full-scale low-rise buildings in the coastal region of South China, a tropic cyclone prone region for investigating the wind effects on low-rise buildings during extreme windstorms. Since the operation of the program in 2006, monitoring of the wind effects on the three instrumented buildings have been performed during more than twenty tropical cyclones, in particular Severe Typhoon Hagupit and Super Typhoon Rammasun with maximum near-ground wind speeds exceeding 60 m/s captured by the measurement stations. This was perhaps the first time in the field of wind engineering to record the wind effects on low-rise buildings during the passages of extreme wind events. Such information is scarce and vary valuable. The damage mechanisms of building's roofs and claddings caused by strong typhoons were clarified and relevant design guidelines were thus proposed for reduction of tropic cyclone wind damages to residential buildings. The measurements and research findings furthered the understanding of the effects of tropic cyclones on low-rise buildings and advanced the current state of wind engineering. This study has been regarded to provide an important contribution to the body of work corresponding to field measurements of tropical cyclone winds and wind loads on low-rise buildings.

In summary, the extensive measurements of the ABL, wind effects on high and low-rise buildings during tropic cyclones as well as subsequent analyzed results provided valuable data and scientific information which is very useful to evaluate the adequacy of codes of practice and to improve structural design to withstand the effects of tropic cyclones.

Apart from conducting the on-site measurement studies briefly introduced above, Prof. Li has also made a series of groundbreaking achievements in the field of computational wind engineering (CWE) based on computational fluid dynamics methods, including: established a general inflow turbulence generator to solve a key problem of accurate simulation of turbulent inlet boundary condition; proposed a new dynamic subgrid-scale model suitable for unstructured or hybrid grids and complex geometry, developed an efficient method for fluid-structure interaction for turbulent flows with high Reynolds number. These new methods and models achieved accurate results of large eddy simulation of the wind effect on super-tall buildings with Reynolds Number in the order of 10^8. In particular, a new simulation approach for evaluation of wind-driven rain (WDR) was proposed based on modified Eulerian multiphase model, which can greatly reduce complexity in evaluations of WDR results and simplifies boundary condition treatments. These research achievements significantly promoted the development of CWE and the practical application of computational fluid dynamics in wind engineering.

In fundamental contribution to wind engineering, Prof. Li carried out a series of wind tunnel studies into the effects of turbulence on pressure fluctuations in separated and reattaching flows. The experiments were conducted in turbulent flows over a much larger

range of turbulence length scale than previous studies to explore the mechanisms of the generation of extreme suctions on bluff bodies under flow separation or conical vortex. It was revealed that how the peak suctions generate and how turbulence affects the generation of the peak suctions. His research works greatly enhanced the understanding of the effects of turbulence on bluff body aerodynamics pertinent to wind engineering applications.

Prof. Li and his collaborators have also carried out research works on bridge aerodynamics. The influence of wind characteristics on the aerodynamic admittances and cross-correlation characteristics of buffeting forces for bridge girders with different sections were investigated through a series of wind tunnel tests, which contributed much to the improvement of the buffeting analysis theory. Their investigation on the coupled vibration of galloping and vortex induced vibration of square bridge towers was conducted and the associated mechanisms were explored, and effective vibration suppression measures were proposed. The vortex induced vibration mechanism of central slotted box girder was studied and the suppression measures were presented, which provided valuable guidelines for the wind-resistant design of super long-span bridges. The aerodynamic loads and wind-induced responses of a number of long-span bridges were investigated by field measurements and wind tunnel tests, which ensured the safe design and construction of these wind-sensitive structures.

Besides Prof. Li's research achievements mentioned above, he has also made significant and sustained contributions to professional practice in wind engineering, structural dynamics, structural health monitoring, and wind environment with over 30 year experience as an engineering consultant. His team has undertaken the wind-resistant design or structural health monitoring of more than 150 high-rise buildings and long-span structures by wind tunnel testing, numerical simulation and field measurement, in which many new methods or strategies proposed by Prof. Li have been applied in engineering practice. For example, an integral optimal design method was proposed by combination of wind tunnel testing results and finite element analysis, to optimize the equivalent static wind loads and structural self-weights through optimization of structural stiffness under the condition of fulfilling constraints for wind-induced responses. This method can significantly reduce construction costs and has been applied to a number of large scale projects. In addition, his contribution to wind engineering and structural engineering extends to service on several national and regional committees such as: the Review of the Code of Practice on Wind Effects in Hong Kong 2004 and the Edit of the National Technical Code for Wind-induced Vibration Control of Building Structures.

In addition to Prof. Li's significant contributions to wind engineering and computational mechanics, he has published more than 100 peer-reviewed journal papers on structural dynamics. His representative works include: proposed efficient structural optimal design methods based on the genetic algorithm and neural networks, especially developed a reduced-order algorithm for structural vibration control as well as a decoupling algorithm and optimal algorithms for the design of active control devices.

In closing, Prof. Qiusheng Li's outstanding achievements made a significant impact in advancing the state-of-the-art in wind engineering, computational mechanics and structural dynamics.

Research in Optical Properties of Materials: Theory & Practice

by David Aspnes, Member EUAS

Short Biography

David E. Aspnes
Department of Physics
North Carolina State University
Raleigh, NC 27695-8202 USA

Distinguished University Professor of Physics, Department of Physics.
Over 350 publications in refereed journals, over 500 publications total.
BSEE, MSEE, University of Wisconsin, Madison, 1960, 1961.
Ph.D., Physics (Mathematics minor), University of Illinois Urbana/Champaign, 1965.
Postdoctoral Research Associate, University of Illinois Urbana/Champaign, 1965-66.
Postdoctoral Research Associate, Brown University, 1966-67.
Member of the Technical Staff, Bell Laboratories, Murray Hill, NJ, 1967-84.
Head of the Interface Physics and Optical Physics Departments, Bellcore, Red Bank, NJ 1984-1992.
Professor of Physics, North Carolina State University, Raleigh, NC, 1992-98.
Distinguished University Professor of Physics, NCSU, 1998-present.
Recognition:
1987: R. W. Wood Prize of the Optical Society of America.
1993: John Yarwood Memorial Medal of the British Vacuum Council.
1996: Frank Isakson Prize of the American Physical Society.
1998: Medard W. Welch Award of the American Vacuum Society.
1998: Elected to the National Academy of Sciences, US.
2011: Mentor Award of the Society of Vacuum Coaters.
2013: Fellow, National Academy of Inventors.
Fellow, American Physical Society, the Optical Society of America, the Society of Photo-Optical Instrumentation Engineers, the American Vacuum Society, and the American Associate for the Advancement of Science.

Research Summary

My research has generally been in the areas of condensed-matter and optical physics, and involves both experiment and theory. In early work I developed low-field electroreflectance, providing the explanation for the anomalously sharp lines seen in electroreflectance spectra and also improving experimental methods of obtaining these data. The accurate values of critical-point energies determined in this way became one of the foundations leading to the development of nonlocal pseudopotential theory and other more accurate methods of calculating the energy band structure of semiconductors.

I next developed the theory and practice of spectroscopic ellipsometry, which is now widely used to determine properties of materials, thin films, surfaces, and interfaces. The advance capitalized on the availability of minicomputers, new at the

time. I used these not only to analyze ellipsometric data but also to acquire them digitally. Digital acquisition improved precision by 3 orders of magnitude, thereby allowing the use of weak continuum sources and making the spectroscopic version of ellipsometry a reality. These data were essential for providing reference spectra for a wide range of materials. More important, work on thin films and otherwise inhomogeneous materials verified the capability of optical spectroscopy and effective-medium theory to obtain structural information on the nanoscale long before plasmonics became a field of its own. The capability of spectroscopic ellipsometry to obtain nanostructural information nondestructively in atmospheric-pressure environments makes it indispensable in current integrated-circuits technology.

Among other results, theoretical work based on limit theorems developed by Bergman and Milton were applied to determine the optimal configuration for maximizing average internal fields in a composite material. In nonlinear optics, the work of Ewald and Oseen, as summarized in their extinction theorem, was shown to be directly applicable to nonlinear optics without requiring self-consistency. This resulted in the anisotropic bond model of nonlinear optics, which has greatly facilitated the interpretation of these data. This is also one of the few examples where the description of a nonlinear response is significantly simpler than its linear equivalent.

Recent contributions include the work of the Aspnes group, where the real-time diagnostic capability of spectroscopic ellipsometry was used to control growth of ZnO by organometallic chemical vapor deposition. This project succeeded in developing a method of growth and processing that yielded p-type material with a carrier concentration of ~10^{18} cm^{-3} at room temperature. The acceptor was shown to be a complex consisting of a Zn vacancy adjacent to a substitutional N atom on an O site, and also involved captured ionized hydrogen. The resulting acceptors have a binding energy of ~130 meV, much shallower than the intrinsically deep (~400 meV) substitutional N on an O site. By solving the long-standing problem of p-type doping in this material, the result provides new opportunities for ZnO in technology. The shallow-acceptor-complex model has implications for other wide-bandgap oxides as well.

Professor Aspnes is presently working with colleagues at Kyung Hee University in Seoul, Korea, on optimizing methods of digitally reducing noise and extracting information from spectra, optical and otherwise. While a wide range of approaches have been designed to do this, a critical assessment remains to be done and improvements are still possible. Improvements are needed particularly in interpolation and scale change, where data obtained linear in wavelength must be converted to spectra linear in energy for analysis. The goal is to develop a simple procedure that does this while minimizing both noise and loss of information.

Mechanical Properties of Lightweight Materials

by Daolun Chen, Member EUAS

Short Biography

Dr. Daolun Chen is a Professor in the Department of Mechanical and Industrial Engineering, Ryerson University, Toronto, Canada. He received his BSc and MSc from Northeastern University (Shenyang, China) in 1983 and 1986, respectively, PhD from the Institute of Metal Research, Chinese Academy of Sciences, 1989, and Dr.rer.nat. from the University of Vienna, Austria, 1993. Prior to joining Ryerson University as an Assistant Professor (2001-2004) and then Associate Professor (2004-2008), Dr. Chen worked as a Post-doc Fellow (1993-1995) and Senior Research Scientist (1995-1997) at the University of Vienna; Research Associate at the University of Manitoba (1997-2000); and Materials and Process Engineer at Bristol Aerospace Ltd., Winnipeg, Manitoba (2000-2001). Dr. Chen has been working in the area of advanced materials and lightweight materials, and their mechanical properties, fatigue, deformation, fracture, microstructural characterization, welding and joining. He has published more than 360 peer-reviewed journal (282) and conference (80) papers, plus additional 190 non-refereed conference papers/abstracts and research reports, including journals "ABC" (Acta Materialia, Biomaterials, Carbon), Journal of Power Sources, Scientific Reports, Scripta Materialia, etc. His research findings have generated an excellent impact, as seen from the citations so far in 8 handbooks/sourcebooks, 97 books or book chapters (where the number of the directly authored/non-edited books is 28), and 119 review papers. His ground-breaking work on metal matrix nanocomposites leads to a well-known method that bears his name, and is twice identified by the Council of Canadian Academies (consisting of the Royal Society of Canada, Canadian Academy of Engineering, and Canadian Academy of Health Sciences) to be one of the top 1% most highly cited paper in his field worldwide. Dr. Chen is an elected Fellow of Canadian Academy of Engineering (FCAE), and a recipient of a number of prestigious awards and honors, including Premier's Research Excellence Award, MetSoc Award for Research Excellence, MetSoc Distinguished Materials Scientist Award, and Sarwan Sahota Distinguished Scholar Award. He is currently an Associate Editor or Editorial Board Member of 28 journals, including Materials; Materials Research Letters; Materials and Design; Materials Science and Engineering A; and International Journal of Fatigue. He has been invited by science reporters in Canada and USA to give interviews and comments on some key scientific breakthroughs published in the journals of Nature and Science. More information could be seen on his web site at http://www.ryerson.ca/~dchen/biography.html.

Examples of Dr. Chen's major contributions to the field of materials science and engineering include the following:

- Dr. Chen has developed and validated several models to predict the strength of nanomaterials and nanocomposites. His pioneering work "Consideration of Orowan strengthening effect in particulate-reinforced metal matrix nanocomposites" (*Scripta Materialia,* 2006, 54, 1321-1326) has received 472 citations (Google Scholar),

including 32 citations in books/book chapters and overview papers, and is listed in the journal's Top 25 "Most Cited Articles" (2006-2011). The method established by Dr. Chen and his graduate student for the prediction of the yield strength of nanocomposites has paved the way for the development of advanced composite materials that are lighter in weight and more durable, translating into important aerospace and automotive applications. This method is now referred to by other researchers as the "Zhang and Chen method," "Zhang and Chen approach" or "Zhang and Chen model" in numerous journal articles and books.

- One of Dr. Chen's most distinguished contributions was a new concept of identifying the effective driving force of fatigue crack propagation in materials by considering the role of the lower portion below the conventional opening load, as reported in his seminal papers: "A model for crack closure" (*Engineering Fracture Mechanics*, 1996, 53, 493-509), and "Contribution of the cyclic loading portion below the opening load to fatigue crack growth" (*Materials Science and Engineering A*, 1996, 208, 181-187). This leads to a more accurate prediction of the lifespan of materials and components. His new closure concept has been described in detail in two important review papers (*Fatigue and Fracture of Engineering Materials and Structures*, 1999, 22, 905-926, and 2003, 26, 1053-1067). Dr. Chen's model has been used by others to successfully predict fatigue lifetime, as quoted herein: "The [Chen *et al.*'s] elastic-wedge model can accurately predict crack development after the infiltration of electroless nickel plating" and "The [Chen *et al.*'s] elastic-wedge model predicted the post-plate crack growth rate more accurately than the rigid-wedge model did." (*International Journal of Fatigue*, 2001, 23, 259-270).

- Dr. Chen is recognized as one of the pioneers in studying cyclic deformation of lightweight alloys. He has identified several new and unique phenomena, including cyclic hardening/softening characteristics, pseudoelastic behavior and twinning/detwinning in magnesium alloys. His research on fatigue of lightweight alloys has successfully been used by Magna International and General Motors for the life prediction of automotive components and for the development of new materials and processes. Dr. Chen and his team are recognized as one of the world's leading research groups in this area. The publication, "Low cycle fatigue properties of an extruded AZ31 magnesium alloy" (*International Journal of Fatigue*, 2009, 31, 726-735) was positioned as No.1 of the journal's "Most Cited Articles" in 2014 and received over 200 citations (Google Scholar).

- Dr. Chen has also developed innovative solid-state welding techniques for joining lightweight aluminum and magnesium alloys. His ground-breaking research has important implications for applications in many manufacturing sectors including automotive and aerospace. He has published more than 70 refereed papers in this area in highly regarded journals, helping position Canada as one of the world's forerunners in the welding and joining of materials. His original paper "Microstructure and tensile properties of friction-stir-welded AZ31B magnesium alloy" (*Materials Science and Engineering A*, 2008, 472, 179-186) has garnered an impressive 268 citations (Google Scholar), including 13 citations in books/book chapters and overview papers. This paper was listed as one of the journal's "Most Cited Articles" (2008-2013). Moreover, three of Dr. Chen's welding papers have been extensively cited in four chapters (or on 22 different pages) of the book *Resistance Welding: Fundamentals and Applications*

(Second Edition, CRC Press, 2012), where 12 figures were directly taken from Dr. Chen's three papers.

Other examples of Dr. Chen's pioneering contributions include: (1) his re-definition of strain hardening capacity (*Scripta Materialia*, 2007, 57, 1004-1007); (2) his new method known as the force balance method to calculate non-dimensional stress intensity factors in fracture mechanics (*Engineering Fracture Mechanics*, 1994, 48, 561-571); (3) the identification of unique core-multishell structures in a friction-stir-welded aluminum alloy (*Journal of Alloys and Compounds*, 2011, 509, 8449-8454) and in a new TiAlNbCr alloy (*Scientific Reports*, 2017, 7, Article number 3483); and (4) the successful fabrication and characterization of iron-containing hydroxyapatite/titanium composites, with the toughening mechanisms published in the top-ranked journal *Biomaterials* (2010, 31, 1493-1501).

Examples of Dr. Chen's recent research work include:

1) **Single and double twin nucleation, growth, and interaction in an extruded magnesium alloy** (F. Mokdad, D.L. Chen, D.Y. Li, *Materials and Design*, 2017, 119, 376-396): The objective of this study was to identify twinning characteristics and mechanisms in an extruded AZ31 magnesium alloy under favorable conditions of profuse $\{10\bar{1}2\}$ extension twinning using in-situ optical microscopy, electron backscatter diffraction, and X-ray diffraction analysis. The propagation of a single twin variant led to a relatively fast saturation of twin nucleation after which the increase in strain was predominantly accommodated by the growth of existing twin lamellas. For distinct twin variants, the intersecting twins led to the confinement of the spaces constrained by the fine twin lamellas. Embryonic twin structures acknowledged theoretically or through atomistic simulations were experimentally observed, including the vanishing of primary $\{11\bar{2}1\}$ embryonic twin via the nucleation and growth of either single or multiple $\{10\bar{1}2\}$ secondary extension twin variants during deformation. Newly identified twin-twin interaction scenarios included the ladder-like and branching-like twinning structures which occurred depending on the applied strain, incoming twin paths, and their impingement on the pre-existing twin boundaries. The formation of the branching-like structures involved three or more non-co-zone $\{10\bar{1}2\}$ extension twin variants where the activation and growth of one variant among them were found to be favored by the external stresses via Schmid factor analysis, as shown in Fig. 1.

2) ***Cymbiola nobilis* shell - Toughening mechanisms in a crossed-lamellar structure** (H.M. Ji, X.W. Li, D.L. Chen, *Scientific Reports*, 2017, 7, Article number 40043): Natural structural materials with intricate hierarchical architectures over several length scales exhibit excellent combinations of strength and toughness. Here we report the mechanical response of a crossed-lamellar structure in *Cymbiola nobilis* shell via stepwise compression tests, focusing on toughening mechanisms, as shown in Fig. 2. At the lower loads microcracking is developed in the stacked direction, and channel cracking along with uncracked-ligament bridging and aragonite fiber bridging occurs in the tiled direction. At the higher loads the main mechanisms involve cracking deflection in the bridging lamellae in the tiled direction alongside step-like cracking in the stacked direction. A distinctive crack deflection in the form of "convex" paths occurs in alternative lamellae with respect to the channel cracks in the tiled direction. Furthermore, a barb-like interlocking

mechanism along with the uneven interfaces in the 1st-order aragonite lamellae is also observed. The unique arrangement of the crossed-lamellar structure provides multiple interfaces which result in a complicated stress field ahead of the crack tip, hence increasing the toughness of shell.

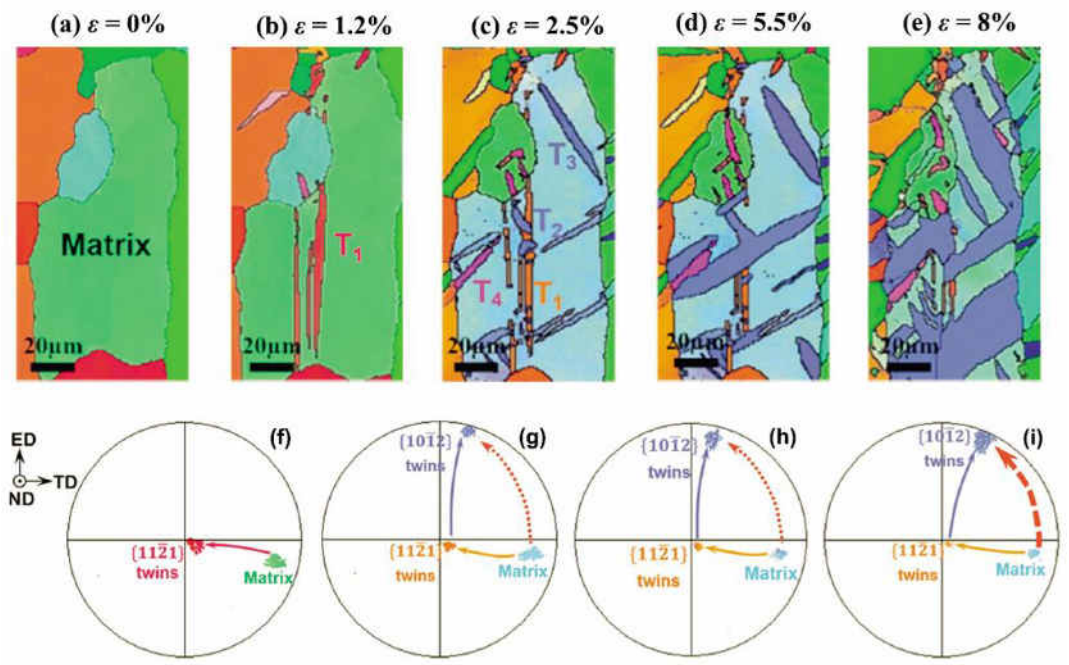


Fig. 1 (a) EBSD orientation maps and the corresponding {0001} pole figures of extruded AZ31 magnesium matrix and twins at different amounts of compressive strain.

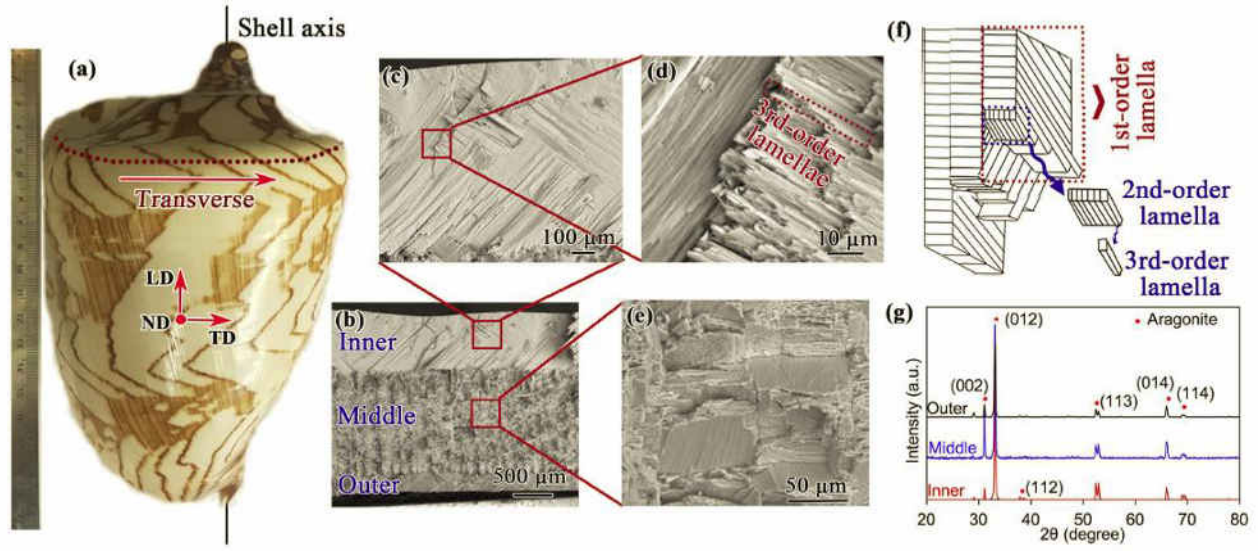


Fig. 2 Overall view (a) and multi-scale hierarchical structures of *C. nobilis* shell, i.e., (b) morphologies on the cross-section of a directly broken sample, (c) and (d) detailed features of the crossed-lamellar structure with the tiled 1st-order lamellae in the inner layer, (e) detailed features of the crossed-lamellar structure with the stacked 1st-order lamellae in the middle layer, (f) schematic drawing of the crossed-lamellar structure, and (g) XRD patterns of the inner, middle and outer layers of *C. nobilis* shell.

Appropriate Technology for Fighting Energy Poverty Developing Countries

by Antonio Lecuona-Neumann, Member EUAS

Short Biography

Antonio Lecuona-Neumann was born in 1953
Full professor in the Universidad Carlos III de Madrid (UC3M), Dep. of Thermal and Fluids Engineering.
Aeronautical Engineer in 1975 and PhD in 1980 with a Thesis on the numerical modelling of the compression with explosives of a micro-ball simulating the laser-driven nuclear fusion of D+T.
A few words can resume his research and teaching activity: Thermofluids and energy.
He has been continuously teaching subjects including: internal combustion engines, energy and environmental engineering, technical acoustics, turbomachinery, combustion, absorption machines, sources of energy and renewable energies, in several universities, either as nominal professor or invited at master and doctorate levels.
Invited Professor at Stanford University from 1986 to 87 in the HTGL laboratory.
He has acted as Vice-chancellor for Engineering studies, Director of Department and sub-director in the Engineering Schools of the Universities where he has being appointed.
Member of the Managing Commission for the establishment of the Universidad Carlos III de Madrid. For his contribution received the highest educational award in Spain "Encomienda de Alfonso X El Sabio"
Editorial board member of Applied Energy and Journal of Solar Energy. Currently, he acts as advisor for the Ministry of Science and Education of Spain as well as for other local governments and private organisations.
He has published two books in Spanish "Turbomáquinas" and "Cocinas Solares" and teaching material for 4 Open-Course-Ware courses in UC3M.
He has tutored 8 doctoral theses, 5 of them with extraordinary official prizes.
Member of the European Advisory Board in July 2005 and of the scientific board in 2006 of the "Centro de Tecnologías Avanzadas para la Combustión Limpia del Carbón" CIEMAT, Spain. This task group was oriented to research in CO2 capture in Spain.
He has contributed to about 100 talks and conferences to national and international congresses.
Author and co-author of 10 national patents.
He is co-author of more than 50 ISI registered papers with "h" factor above 20. Around 1.400 cites.
He has participated in 8 European Commission competitive research projects PIVNET, PIVNET2, EUROPIV, EUROPIV2, LSP, LOWNOXIII, COJEN and HOT, as well as in many industrial projects.

The World Energy consumption of biomass reaches about 10% of total, the most consumed "Renewable Energy". The reality is this consumption carries on deforestation and biodiversity reduction. About 90% of biomass in in form of woody product. It is mainly burned for heat production. It forms up to 90% of the primary energy consumption of some third world countries, primarily used for cooking and indoor space heating.

Cooking can be produced burning firewood at a much higher efficiency than nowadays, using improved cookstoves that would reduce consumption to half. These cookstoves can be manufactured locally using the simplest techniques and local materials, such as clay. More elaborate types require ironwork and soldering. The resultant benefits are huge, as not only biomass will be preserved but also the air pollution, both indoors and outdoors, will be much reduced. Burning biomass produces much flying particles and nitrogen

oxides, besides other concomitant pollutants. These contaminants cause several million premature deaths annually, according to the World Health Organization.

A complementary technique that can alleviate pressure on firewood is solar cooking. Also using simple techniques the sun can cook food, prepare sanitary hot water and sterilize medical apparatus. One exponent of the scientific activity on solar cooking is the recent congress CONSOLFOOD 2018, in Faro, Portugal, http://www.consolfood.org/ . The non-profit organization Solar Cookers International is another example. A recent book on solar cooking scientific principles can be obtained for free:

Cocinas solares. Fundamentos y aplicaciones

By: Antonio Lecuona. Editorial Marcombo, ISBN: 9788426724038, 2017.
http://marcombo.info/ code for free download:cocinas1
Some other recent publications are those by the author:
Antonio Lecuona-Neumann, José I. Nogueira and Mathieu Legrand, Chapter 13 - Photovoltaic Cooking, In Advances in Renewable Energies and Power Technologies, edited by Imene Yahyaoui, Elsevier, 2018, Pages 403-427, ISBN 9780128129593, https://doi.org/10.1016/B978-0-12-812959-3.00013-7

Antonio Lecuona-Neumann, Pedro A. Rodríguez-Aumente, Mathieu Legrand., Chapter 16 - Solar Cooking For in Sustainable Energy Technologies (Hardcover) edited by Eduardo Rincón-Mejía and Alejandro de las Heras, Pages 255- CRC Press ISBN: 978-1-138-03438-9.

Solar cookers just uses four mechanisms to reach cooking temperatures:

1. Optical concentration, using mirrors or lenses.
2. Sun ray absorption by a black surface.
3. Greenhouse effect. The pot is covered by an enclosure transparent to visible light but opaque for infrared spontaneous radiation, thus forming a light trap. Moreover, if the enclosure is impervious the surrounding heated air is enclosed, thus reducing the convective losses.
4. Reducing water evaporation that carries much latent heat.

A recent addition to the conventional direct use of the sun rays to produce heating is PV cooking. This possibility is enabled by the dramatic price reduction of solar panels. A family can cook on a sunny day with a single 300 W peak power PV panel, costing over-the counter 200 €. The remaining equipment allowing to cook in an indoor kitchen can amount 100 € more. This is a huge amount for the poor families. But the electricity will be for free during more than 20 years. Financing would be possible by the side benefits; this is, the possibility of charging mobiles, computers and smartphones with the same PV panel. This is with no electrical grid deployment. Actions implementing these tiny renewable electricity producers are the seed of future smart grids to share electricity and possibly digital information. One main barrier now is electricity massive storage using batteries. Their high cost, short duration and pollution when scrapped discourages deployment in the developing countries. Solar cooking with no sun is still possible resourcing to thermal storage. Nano-scale batteries, such as those in luminaires and phones are already appropriate.

Near half of the agricultural production worldwide is lost on a continuous bases because of biological degradation. In developing countries much can be gained if food preservation techniques using autonomous energy can be applied. Not only hunger can be fought but also poverty and food security. Refrigeration and freezing requires sophisticated heat pumps driven by electricity. Even though a freezer requires a modest power, in the range of 30 to 300 W at the family scale investment on the PV panels and freezer can add up to around 500 €. An alternative is dehydration or more commonly, drying.

Open sun drying has been practiced by humanity for millenniums. Safer and better quality products can be obtained by solar driers. In them a solar air collector heat air up to 60 ºC and downstream it dehydrates the moist material disposed over wire mesh trays inside a cabinet. The low temperatures allow the solar collector to be made with low-cost transparent material, but in any case imported as it must be made of plastic or glass.
The necessary hot air current can be produced naturally by buoyancy forces, otherwise a PV panel for motoring an air draft fan is necessary.

Although the physical principles of dehydration and more particularly air convection drying have been much studied the physical principles and what technologies are appropriate to remote and isolated communities have not been analyzed so deeply. Using only solar thermal energy is a challenge for drying. The 1D, downstream z, low Mach number motion of a mixture of air $\boldsymbol{a}$ and humidity $\boldsymbol{w}$ with mass fraction $\boldsymbol{y}$, with mixed velocity $\boldsymbol{v}$ inside a $\boldsymbol{\theta}$ tilted conduit of cross-section A_z, wet perimeter $\boldsymbol{p}$, is governed by the equations:

Continuity: $$\dot{m} = \rho v A_z = \dot{m}_a + \frac{\mathbf{d}\dot{m}_w}{\mathbf{d}z}\mathbf{d}z \; ;$$

Momentum: $$A_z \frac{\mathbf{d}p}{\mathbf{d}z} + \rho v A_z \frac{\mathbf{d}v}{\mathbf{d}z} = -P\tau_w - A_z \rho g \sin\theta$$

The wall shear stress is commonly correlated using Darcy friction coefficients. But unfortunately there is not much information available for the precise flow layouts present in solar convective driers, especially to near laminar Reynolds numbers.

Energy for flow:

Energy for non-solarized charge: $$m_w c_{ch} \frac{\mathbf{d}T_{ch}}{\mathbf{d}t} = \alpha_w A_{ch} (T - T_w)$$

This equation is frequently ignored because the characteristic time for heating the charge is much smaller that the time for drying so that generally $T = T_w$ is assumed.

Equation of state of mixture in equilibrium:

$$\frac{p}{\rho} = R_g T \; ; \begin{Bmatrix} \rho^{-1} \\ R_g \\ c_p \end{Bmatrix} = y \begin{Bmatrix} \rho_w^{-1} \\ R_{gw} \\ c_{pw} \end{Bmatrix} + (1-y) \begin{Bmatrix} \rho_a^{-1} \\ R_{ga} \\ c_{pa} \end{Bmatrix} ; \; p = p_w + p_a \, .$$

Mass transfer rate equations:

Fist constant rate regime: It appears for high water containing charge materials. The mass transfer rate through surface area A_{ch}:

$$\dot{m}_w = k_w \, A_{ch} (p_w - p_{we}) \quad (1)$$

The equilibrium water pressure at the charge/air interphase p_{we} is generally obtained by experimental means. Generally corresponds to the saturation water vapor into air excepting the water activity is smaller than one, owing to the presence of solutes: $p_{we} = p_s a_w$.

Second decreasing rate regime: During drying, after a critical point this regime appears. Eq. (1) is substituted by the ratio of water content of the charge pieces or radius $\boldsymbol{r}$, coming from a simplified solution of the Fick law:

$$\frac{m_{wch}}{m_{win}} = A_{chin}\left(\frac{1+uy_{dB}}{1+uy_{dBin}}\right)^{\frac{2}{3}} \exp\left(-\frac{D_{eff}t}{r^2}\right) \quad (2)$$

Eq. (2) takes into consideration a linear shrinkage coefficient u with instantaneous moisture content y_{db} and initial y_{dBin} and initial contact area A_{chin} of the charge pieces. Eq. (2) is valid for spherical and cylindrical shapes, but can be extended for other shapes.

The pieces material effective diffusion coefficient D_{eff} is generally obtained experimentally as the mechanisms of water migration are complex and sometimes of overlapping regimes. It is well accepted that it has an activation energy $\boldsymbol{E}$:

$$D_{eff} = d\exp\left(-\frac{E}{RT}\right)$$

Typically $E \gg RT$, so that a linearization can be safely assumed. A non-trivial effect of moisture content y_{wdB} is typically encountered. Unfortunately, several experimentally obtained correlations for D_{eff} include the positive effect of the flow velocity $\boldsymbol{v}$, what is extraneous to the dominance of the internal resistance to moisture migration.

Heat transfer: $\dot{q} = S - a_1(T - T_{atm}) - a_2(T - T_{atm})^2$ -; (3)

Applied power: $\dot{w}$ prescribed, e. g. a fan

$\boldsymbol{S}$ stands for the impacting solar irradiance and degrades mechanical energy, a_1 and a_2 stand for empirical heat losses to ambience. α_w and k_w are the heat and mass transfer coefficients charge/flow. For the case that the internal mass transfer is dominant (decaying regime of drying)

The boundary conditions are an inlet from atmosphere with possible wind ram effect and a subsonic outlet condition with possible wind ram effect at a different geographical height.

The various processes present in solar drying makes the successful resolution of the set of equations complex, even being 1D. The complexity is not mathematical, but of using representative enough empirical values. Because of this, its calibration is not simple.

The modeling effort offers some benefits. One is the possibility of optimizing the design. The immediate issue is that a low value of $\boldsymbol{v}$ will increase the air flow temperature, increasing the rate of water evaporation, but decreasing the convective heat and mass transfer with the charge pieces.

Another issue is the algorithm for acting on a PV fan installed for boosting the efficacy of the solar drier. The appropriate size is something important owing to the high cost of the PV panel, in front of the high loss of a rotten crop because of a too large bad weather period.

A more far reaching issue would be the optimization of the design of a thermal storage embedded into the solar collector, making its cost appropriate to every location and allowable cost. Whether a rock or sand based design is effective enough in front of a Phase Change Material (PCM), of a higher cost is something that a sensible modelling can discriminate before any investment, both in capital and in human resources is endeavored.

In addition of these technical issues, that are easily reachable in our technology developed societies, there are important issues to be successfully accomplished to make even the most appropriate technology not to fail. Training of traveling cooperants, training of in-situ cooperants and education of the communities and social agents to whom the benefit is destined is of paramount importance and a non-negligible effort in planning, direct action and project following and evaluation. Many program failures could be attributed to errors in those dimensions.

Innovative Energy Research & Technology

by Mohsen Assadi, Member EUAS

Short Biography

Present positions

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

Previous position

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

Education

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

Courses and education

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

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

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

PhD Courses

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

Main fields of competence

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

Project leadership

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

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

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

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

Prof. Assadi's energy research at University of Stavanger

The global energy industry has been through a tremendous change during the last decades. The ever-increasing share of intermittent renewable energy in the national grids and the political decision concerning reduced CO_2 emission from power sector has changed the power market considerably.

The research activities within the energy research group at University of Stavanger (UiS) have been focused on Energy System Integration, Analysis and Optimization to support better understanding of the current transition of the energy system towards smart distributed energy systems with larger penetration of the intermittent renewable energy.

Developing validated component and system models using real plant data has enabled the research group to carry out system studies for large centralized power plants as well as distributed small-scale units, utilizing both fossil and non-fossil-based fuels. Access to validated models provides opportunity for identification of possible system configurations and layouts that can enable high flexibility, high efficiency and low emissions. Research activities of the energy research group at UiS have followed the international development trend mentioned above, with focus on method and tool development. The short presentation given below provides a general overview of the R&D activities conducted in the recent years.

The current trends towards utilization of data driven modeling (also called digital twins) and artificial intelligence, covering instrumentation, data gathering/storage and data analytics have been the corner stones of the methods and tools developed for the last decade. Data from locally operated units, such as micro gas turbines, internal combustion engines, fuel cells, as well as large-scale commercial power plants have been utilized for optimization of the plant instrumentation and condition monitoring to facilitate predictive and condition based maintenance, enabling higher availability and better plant economy.

Given the fact that gas turbine based power plants, with and without carbon capture,

have been in focus during late 1990's and early 2000 due to their high flexibility, high efficiency and low emissions, large efforts were dedicated to develop tools for analysis and optimization of these plants. The high efficiency achieved required costly components such as heavily air-cooled turbine blades, which motivated use of more sophisticated monitoring systems. Therefore, in collaboration with power industry and plant manufacturers various methods and tools, utilizing real time plant data, were developed and evaluated to support both the component manufacturers, who have access to detailed component data, and the power producers who have access to the plant operational data. A combination of thermodynamic- and data driven models were used for this purpose with very good results [1-8].

The promising results of the data driven modeling resulted in more focused research on use of artificial intelligence approaches, based on Artificial Neural Networks (ANN). Monitoring tools were developed and successfully implemented, enabling early warning systems for condition-based maintenance. Considering a future energy system containing numerous units of different kinds, distributed over large geographic areas, one will need local monitoring systems to maintain their performance and provide condition based maintenance to enable economic viability of the energy system [9-13].

The North Sea region has been identified as the energy hub of Europe, with both large investments in petroleum infrastructure and large potential for renewable energy. Within a EU-financed project, European North Sea Energy Alliance (ENSEA), the potential for an integrated energy system in the North Sea region was investigated. For more info and access to the reports generated within the frame of the project the readers are referred to the: http://www.ensea.biz/downloads/

As follow up of the findings within the ENSEA project, the future development of the North Sea region as European energy hub will be investigated in an ongoing EU-project, Energy System in Transition (ENSYSTRA). Six partner countries, 15 PhD students and several industrial partners are involved in this multi-disciplinary research project, aiming at providing an integrated simulation environment for potential studies and decision support for future development of the North Sea region https://ensystra.eu/ .

The European vision of reduced dependency on import fuels resulted in increased interest for clean coal technology for power generation, based on integrated gasification combined cycle plants with pre-combustion CO_2 capture. The energy research group at UiS were involved in a FP7 EU-funded project, H_2-IGCC, where the UiS group was responsible for system integration and techno-economic evaluation of IGCC plants in a comparative study versus natural gas fueled combined cycles and super-critical pulverized coal plants. The project was successfully completed and besides system modeling and analysis tools, a full-scale premixed burner for hydrogen fuel was developed and tested. However, need for flexible generation units that can match the increased share of intermittent renewable energy was opposite to characteristics of the IGCC plants, which are most suitable for base load operation [14-16].

Although IGCC plants were not the most suitable option for the future energy system in the EU, clean coal could play an important role in countries such as Poland and India, due to their heavy dependency on coal for power generation in the coming decades. Therefore, within a collaborative project with Indian partners from the west Bengal the need for clean coal technologies and thereby IGCC technology was highlighted as an interesting technology for Indian energy market. The interest for IGCC technology provides opportunity for knowledge transfer that could have impact on CO_2 reduction at a global level [17-18].

Increased share of intermittent renewable energy, i.e. wind and solar energy, in the

European energy system in combination with growth of number of electrical vehicles have increased the interest and need for distributed power generation and the impact analysis on the electrical grid. Using biogas as fuel backed up with natural gas as transfer fuel, in small-scale power conversion technologies, namely micro gas turbine, internal combustion engine and solid oxide fuel cells was investigated both experimentally and theoretically within a nationally funded project. This resulted in development of validated mathematical models as well as data driven ANN based models that can support further development of the distributed fuel flexible technologies [19-26].

CO_2 capture and storage have been considered as an important measure to reach the global CO_2 target. The political support and commercial interest in capture technologies have been changing during the last decades. The R&D activities concerning development of validated methods and tools have been part of the activities of the energy group at UiS. The model development and investigation of innovative cycles have been carried out in collaboration with other research groups. Experimental data from various test rigs, especially in collaboration with the UK based Sheffield University, were used for pilot studies aiming at evaluation of techno-economic potential of various capture alternatives [27-35].

Utilization of low temperature heat sources and industrial waste heat for heat and power generation has been studied by the UiS energy group to provide better understanding of the economic potential of waste heat utilization. Validated models for waste heat utilization from aluminum industry were developed based on experimental data from test cell setup [36-40]. The current development in this field is focusing on utilization of geothermal energy and the knowledge transfer from the petroleum sector, especially drilling technology and well integrity, which has resulted in establishment of a multidisciplinary research group at UiS, consisting of experts from petroleum engineering, material science, energy conversion technology and socio-political science. Preliminary results of this multidisciplinary research initiative are expected in 2018.

Refernces

1. Palmé T., Waniczek P., Hönen H., Assadi M., Jeschke P., “Compressor Map Prediction by Neural Networks”, Journal of Energy and Power Engineering, Volume 6, Number 10, pp. 1651-1662, October 2012.
2. Jordal K., Assadi M., Genrup M., “Variations in Gas-Turbine Blade Life and Cost due to Compressor Fouling – a Thermoeconomic Approach”, International Journal of Applied Thermodynamics, Mars 2002.
3. Palme T., Breuhaus P., Assadi M., Klein A., Kim M., “New Alstom monitoring systems leveraging artificial neural network technology”, ASME Turbo Expo 2011, GT2011-45990, Vancouver, Canada.
4. Palme T., Breuhaus P., Assadi M., Klein A., Kim M., “Early warning of gas turbine failure by nonlinear feature extraction using an auto-associative neural network approach”, ASME Turbo Expo 2011, GT2011-45991, Vancouver, Canada.
5. Möller B. F., Assadi M., “CO2-free power generation in combined cycles – integration of post-combustion separation of carbon dioxide in the steam cycle”, Journal of Energy.
6. Möller B. F., Arriagada J., Assadi M., Potts I., “Optimisation of an SOFC/GT system with CO2 Capture”, Journal of Power Sources 131 (2004), pp. 320-326, ELSEVIER.
7. Sipöcz N., Tobiesen F.A., Assadi M., “Natural gas combined cycle power plants with CO2 capture-Opportunities to reduce cost”, International Journal of Greenhouse Gas Control, 2011.
8. Sipöcz N., Jonshagen K., Assadi M., Genrup M., ”Novel high-performing single-pressure combined cycle with CO2 capture”, Journal of Engineering for Gas Turbines and Power, Vol. 133/041701, April 2011.
9. Nikpey H., Assadi M., Breuhaus P., Mørkved P. T., “Experimental evaluation and ANN modeling of a recuperative micro gas turbine burning mixtures of natural gas and biogas”, Applied Energy 2014; 117 (2014) 30–41.
10. Nikpey H., Mansouri M., Breuhaus P., Assadi M., “Performance analysis of a biogas-fueled micro gas turbine using a validated thermodynamic model”, Applied Thermal Engineering 2014; 66 (2014) 181-190.
11. Mesbahi E, Arriagada J, Assadi M, Ghorban H: "Diesel Engine Fault Diagnosis by Means of ANNs: A Comparison of Two Methods". Journal of Marine Design and Operations, No B6 (2004), ISNN 1476-1556, pp.
12. Nikpey H., Assadi M., Breuhaus P., “Experimental investigation of the performance of a micro gas turbine fueled with mixtures of natural gas and biogas”, IMECE2013-64299, Proceedings of ASME IMECE 2013, San Diego, USA 2013.
13. A. Safari, H. Nikpey, K. Haji H., M. Assadi, “Application of an Experimentally Validated High-dimensional Surrogate Model to Performance Prediction of a CHP Unit”, Energy Procedia 142 (2017) 1106–1111

14. Mansouri Majoumerd, M., Assadi M. "Techno-economic assessment of fossil fuel power plants with CO2 capture – Results of EU H2-IGCC project", International journal of hydrogen energy, Volum:39 Issue:30, pp. 16771 -16784, 2014.
15. Nikpey H. Assadi M., Breuhaus P., "Development of an optimized artificial neural network model for combined heat and power micro gas turbines", Journal of Applied Energy, 108 (2013) 137–148.
16. Razbani O., Wernhus I., Assadi M., "Experimental Investigation of Temperature Distribution over a Planar Solid Oxide Fuel Cell Applied Energy", Journal of Applied Energy, 105 (2013), pp. 155-160.
17. Severson H., Assadi M., "Modelling of overpotential in an anode-supported planer SOFC using a detailed simulation", Journal of Fuel Cell Science and Technology OCTOBER 2011, Vol. 8 / 051021-1.
18. Selimovic A., Kemm M., Torisson T., Assadi M., "Steady State and Transient Thermal Stress Analysis in planar Solid Oxide Fuel Cells", Journal of Power Sources.
19. U. Ali, C. Font-Palma, H. Nikpey, M. Mansouri, M. Akram, K. Finney, T. Best, N. Mohd Said, M. Assadi, M. Pourkashanian, "Benchmarking of a micro gasturbine model integrated with post-combustion CO2 capture", Energy 126 (2017) 475-487,http://dx.doi.org/10.1016/j.energy.2017.03.040.
20. Mansouri Majoumerd, M., Nikpey H., Assadi M., Breuhaus P., "Micro gas turbine configurations with carbon capture - Performance assessment using a validated thermodynamic model", Applied thermal engineering [1359-4311], 2014 Volume:73, book:1, pp:170 -182.
21. Liu Chunyang; Chen Gang; Sipøcz Nikolett; Assadi Mohsen; Bai Xue-Song. "Characteristics of oxy-fuel combustion in gas turbines", Applied Energy 2012 ;Volum 89.(1) pp. 387-394
22. Sipöcz N., Tobiesen F.A., Assadi M., "The use of artificial neural network models for CO2 capture plants", Applied Energy vol. 88, Issue 7, pp. 2368-2376, July 2011.
23. J. Smrekar, D. Pandit, M. Fast, M. Assadi, Sudita De, "Prediction of power output of a coal-fired power plant by artificial neural network", Journal of Neural computation and Applications, DOI 10.1007/s00521-009-0331-6, ISSN 0941-0643, Volume 19, Number 5, 2010.
24. Sipocz N., Assadi M., "Combined Cycles With CO2 Capture: Two Alternatives for System Integration", J. Eng. Gas Turbines Power, June 2010, Volume 132, Issue 6, 061701 (6 pages) doi:10.1115/1.4000122.
25. Fast M., Assadi M., De S., "Development and multi-utility of an ANN model for an industrial gas turbine", Journal of applied energy, vol. 86, Issue 1, pp. 9-17, January 2009.
26. Smerekar J., Assadi M., Fast M., Kustrin I., De S., "Development of artificial neural network model for a coal-fired boiler using real plant data", Energy 2009, volume 34, issue 2, year 2009, pp. 144 - 152.
27. De S., Kaiadi M., Fast M., Assadi M., "Development of an artificial neural network model for the steam process of a coal biomass co-fired Combined Heat and Power (CHP) plant in Sweden", Journal of Energy, Energy 32 (2007) 2099–2109.
28. Y. Mollaei Barzi, M. Assadi, K. Parham, "A waste heat recovery system development and analysis using ORC for the energy efficiency improvement in aluminium electrolysis cells", International Journal of Energy Research, DOI: 10.1002/er.3940, Nov. 2017.
29. K. Parham, M. Assadi, "A Parametric Performance Analysis of a Novel Geothermal Based Cogeneration System", Volume 2, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018
30. Mondal, S., De, S. and Assadi, M. (2017): Waste heat recovery from flue gas containing SO2 through CO2 based combined power and refrigeration cycle, Journal of Energy and Environmental Sustainability, 3, 51-55.
31. Y. M. Barzi, M. Assadi, "Evaluation of a Thermosyphon Heat Pipe Operation and Application in a Waste Heat Recovery System", Experimental Heat Transfer, DOI 10.1080/08916152.2014.913089, pp. 493-510, Volume 28, Issue 5, 2015
32. Mollaei Y., Assadi M., "Heat transfer and thermal balance analysis of an aluminum electrolysis cell side lines: A heat recovery capability and feasibility study", IMECE2013-64358, Proceedings of ASME IMECE 2013, San Diego, USA 2013.
33. Fast M., Assadi M., De S., "Development and multi-utility of an ANN model for an industrial gas turbine", Journal of applied energy, vol. 86, Issue 1, pp. 9-17, January 2009.
34. Smerekar J., Assadi M., Fast M., Kustrin I., De S., "Development of artificial neural network model for a coal-fired boiler using real plant data", Energy 2009, volume 34, issue 2, year 2009, pp. 144 - 152.
35. De S., Kaiadi M., Fast M., Assadi M., "Development of an artificial neural network model for the steam process of a coal biomass co-fired Combined Heat and Power (CHP) plant in Sweden", Journal of Energy, Energy 32 (2007) 2099–2109.
36. Y. Mollaei Barzi, M. Assadi, K. Parham, "A waste heat recovery system development and analysis using ORC for the energy efficiency improvement in aluminium electrolysis cells", International Journal of Energy Research, DOI: 10.1002/er.3940, Nov. 2017.
37. K. Parham, M. Assadi, "A Parametric Performance Analysis of a Novel Geothermal Based Cogeneration System", Volume 2, ISBN 978-981-10-8392-1, ISSN 1865-3529, 2018
38. Mondal, S., De, S. and Assadi, M. (2017): Waste heat recovery from flue gas containing SO2 through CO2 based combined power and refrigeration cycle, Journal of Energy and Environmental Sustainability, 3, 51-55.
39. Y. M. Barzi, M. Assadi, "Evaluation of a Thermosyphon Heat Pipe Operation and Application in a Waste Heat Recovery System", Experimental Heat Transfer, DOI 10.1080/08916152.2014.913089, pp. 493-510, Volume 28, Issue 5, 2015
40. Mollaei Y., Assadi M., "Heat transfer and thermal balance analysis of an aluminum electrolysis cell side lines: A heat recovery capability and feasibility study", IMECE2013-64358, Proceedings of ASME IMECE 2013, San Diego, USA 2013.

Structural Phenomenon of Concrete Elements at Limit States

by Yuri Ribakov, Member EUAS

Short Biography

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

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

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

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

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

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

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

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

2000 Abraham and Miriam Gutwirth Research Award.

2013 Reviewing Excellence Award, Engineering Structures, Elsevier.

2014 Outstanding Reviewer Award, Engineering Structures, Elsevier.

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

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

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

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

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

Reinforced concrete (RC) is a composite material that has minimum two components, one of which has higher strength (steel) compared to other (concrete). Similar materials are also ferro-cement, two- (or multi-) layer RC elements, retrofitted RC structures, etc. The authors have payed attention to a structural phenomenon that many design features at ultimate limit state (ULS) of a structure (or its element) are twice higher (or lower) then at initial loading state. This phenomenon is evident for material properties, structure (or its elements), static and/or dynamic structural response. The phenomenon is based on two ideas**:** quasi-isotropic state of a structure at ULS and mini-max principle [1, 2]. This phenomenon is supported by numerous experimental and theoretical results, obtained for various structures, like beams, frames, spatial structures and structural joints under static or/and dynamic loadings.

It should be mentioned that the structural phenomenon is just a private case of the following global concept. According to the Torah, "Thou shalt love thy neighbour as thyself" [3], Figure 1 [4]. There are two sides in this context – the person, N_1, and its neighbor, N_2. According to the Torah, each person is unique and therefore all people are equal, hence N_1 is not grater and not less than N_2, or $N_1 = N_2 = N$ and $N_1 + N_2 = 2\,N$.

Figure 1. "You shall love your neighbor as yourself" [4].

The above-mentioned Torah statement means that the overall load is redistributed and each person carries half of the entire load. It forms a direct basis not just for humanity, but also for structures. The phenomenon is that values of some parameters of the structure that are measured experimentally under static or/and dynamic loadings increase or decrease by about a factor of two. Therefore, an alternative name of this phenomenon is doubling of structural design parameter at ULS.

For example, the Figure 2 presents dependence of dominant vibration mode frequency of a 1:10 scaled model of a 24 × 24 m RC roof shell vs. load ratio, q / q_{ul} [5]. Here q is the live load (the value of q is varied from 0 to q_{ul}) and q_{ul} is its ultimate value. As it follows from the Figure, at the ULS (q = q_{ul}) the above - mentioned parameter decreases twice, relative to its initial value.

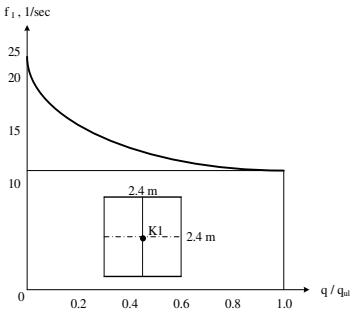


Figure 2. Dominant technical frequency, f_I, vs. load ratio, q / q_{ul}.

Figure 3 illustrates a problem of increasing residual deflections in a full scale 24×24 m RC roof shell under static load and additional vertical seismic excitation. The selected for analysis earthquake records include high-, medium- and low frequency motions. The dependence of residual deflections on damping ratio was studied. The initial static deflection in the middle of the shell, w, equals 2.2 cm. The damping ratio, ξ, varied from 0 to 12%. For a high frequency earthquake (curve 1) the residual deflections are accumulated very intensively and for ξ=0 reached 4.4 cm, which is two times higher, compared to the static value. A similar result was obtained for a medium frequency earthquake (curve 2), for which the residual deflection equals 3.9 cm. However, for a low-frequency earthquake (curve 3) the increase in residual deflections is lower. It is because the dominant frequency of the shell is high and comparable with that of a high-frequency earthquake.

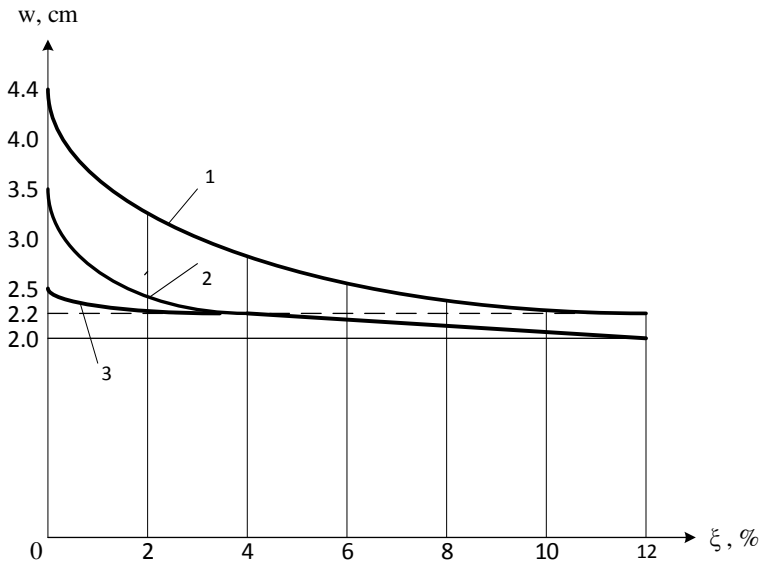


Figure 3. 24×24 m shell deflection vs. damping ratio for various ground motions: 1–high frequency earthquake, 2–medium frequency earthquake, 3–low frequency earthquake.

Four-point static tests in ultimate stages show that steel fibers increase the deflections in the middle-span of a high strength concrete bending element approximately twice [6]: the deflections in beams made of concrete class C140 were 44 and 84 mm without and with steel fibers, respectively. For beams made of concrete class C200 adding steel fibers has increased the deflections from 33 to 59 mm. As in the previous examples, the fact of doubling the middle-span deflections was not emphasized.

It is logically to analyze the structural phenomenon from the following three different groups of experiments: investigation of structural concrete at material level; behavior of RC structures and elements under static loads; response of RC structures and elements to dynamic loads.

Using high strength concrete in construction became very popular in recent decades. At the same time, in spite that concrete compressive strength increases with concrete class, the mean value of concrete tensile deformations, ε_{ctm}, reaches its maximum for concrete class C 70 and remains constant for higher concrete classes. The maximum value of ε_{ctm} is about $1.2 \cdot 10^{-4}$, and for the lowest concrete class it is about $0.6 \cdot 10^{-4}$. It is one of the structural phenomenon evidences, as $\varepsilon_{ctm\,\max} / \varepsilon_{ctm\,\min} = 2$.

As an extension of this idea, let us discuss the relation between the displacements and Poisson deformations under ultimate load and after unloading of two-layer beams consisting of normal and fibered high strength concrete in tensile and compression zones, respectively. Following experimental results for full-scale 3 m beams [7], the mid span displacement under the ultimate load was 35 mm and the residual deflection – about 18 mm. The corresponding Poisson deformations were about $0.65 \cdot 10^{-3}$ and $0.32 \cdot 10^{-3}$. A similar behavior was observed for horizontal shear deformations between the concrete layers. The maximum deformations under the ultimate load were $2.7 \cdot 10^{-3}$, whereas the residual ones were about $1.25 \cdot 10^{-3}$.

Increasing the load, acting on cylindrical concrete specimens with different steel fibers contents (from 0 to 60 kg/m^3), yields increase in Poisson coefficient, ν [8]. The optimal fiber content is 30 kg/m^3. Following the experimental data, in specimens without fibers $\nu_{min\ 0} = 0.11$ and $\nu_{max\ 0} = 0.22$. In specimens with optimal fibers content $\nu_{min\ 30} = 0.22$ and

$\nu_{max\ 30} = 0.44$. The ratios $\frac{\nu_{min\ 30}}{\nu_{min\ 0}} = \frac{\nu_{max\ 30}}{\nu_{max\ 0}} = 2$, $\frac{\nu_{max\ 30}}{\nu_{min\ 30}} = \frac{\nu_{max\ 0}}{\nu_{min\ 0}} = 2$ demonstrate that, like in case of longitudinal deformations, also for transverse ones the parameters are doubled.

Disengagement of concrete braces in a six story RC braced frame leads to a system with variable stiffness [9]. Seven structural static schemes, from fully braced to unbraced, were analyzed (three of them are shown in Figure 4). The dominant natural vibration periods were $T_1 = 0.248$ s, $T_4 = 0.433$ s and $T_7 = 1.037$ s. Thus, $T_4 / T_1 = 0.433 / 0.248 = 1.75$; $T_7 / T_4 = 1.037 / 0.433 = 2.39$. In this case also the average difference in the natural vibration periods is 2.07.

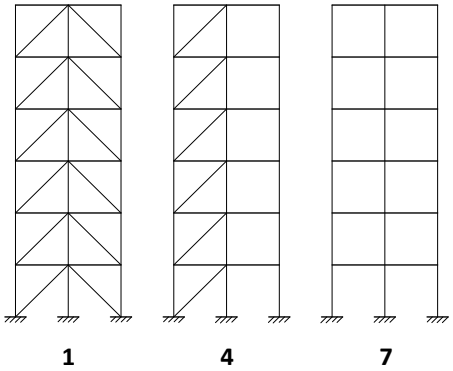


Figure 4. Changes in the basic frame scheme under growing horizontal dynamic loading.

The structural phenomenon enables to predict the ULS of the building or appropriate safety factor to this state; to assess the limit changes of strength and deformation parameters in buildings before beginning their real design; to solve strengthening problems of a building; to find the limit values of steel fibers; to evaluate the seismic resistance of a structure, i.e. the level of structural load bearing capacity under a strong earthquake; to reveal the stage, when the structural static scheme is changed.

The results of this study provide valuable indicators for experiments planning, estimation of structural state, evaluating possibilities of retrofitting, etc. From the mathematical viewpoint, the phenomenon provides additional equation(s) that enable to calculate parameters, usually obtained experimentally or using some coefficients. Therefore, using this phenomenon can lead to developing proper design concepts and new RC theory, in which the number of empirical design coefficients will be minimal.

Acknowledgements

This article was written in cooperation with Prof. I. Iskhakov

References

1. I. Iskhakov and Y. Ribakov, Optimization of steel ratio in cement based composite bending elements. 13th International Conference "Mechanics of Composite Materials MSM 2004", May 16-20 2004, Riga, Latvia.
2. I. Iskhakov and Y. Ribakov, *Ultimate Equilibrium of RC Structures using Mini-Max Principle*, Nova Science Publishers, Inc., New York, 2014.
3. Torah, Leviticus, Vayikra, 19:18.
4. Internet resource https://he.wikipedia.org/wiki/%D7%95%D7%90%D7%94%D7%91%D7%AA_%D7%9C%D7%A8%D7%A2%D7%9A_%D7%9B%D7%9E%D7%95%D7%9A, accessed on September 24, 2015.
5. I. Iskhakov. *Design and Construction of RC Shells for Seismic Zones*, Maorif, Dushanbe, 1983 (in Russian).
6. J. Magnuson and M. Hallgern, Reinforced high strength concrete beams subjected to air blast loading. In: N. Jones and C.A. Brebbia (Eds.), *Structures under shock and impact*, 8-th ed., vol. VIII. WIT Press; 2004.
7. I. Iskhakov, Y. Ribakov, K. Holschemacher and T. Mueller, Experimental investigation of full-scale two-layer reinforced concrete beams, *Mechanics of Advanced Materials and Structures*, 21, 273-283, 2014.
8. K. Holschemacher, I. Iskhakov, Y. Ribakov and T. Mueller, Laboratory tests of two-layer beams consisting of normal and fibered high strength concrete: ductility and technological aspects, *Mechanics of Advanced Materials and Structures*, 19, 513-522, 2012.
9. I. Iskhakov and Y. Ribakov, Experimental and numerical investigation of a full-scale multistory RC building under dynamic loading, *The Structural Design of Tall and Special Buildings*, 14, 299-313, 2005.

Innovative Improvements in Vascular Biology

by Yihai Cao, Member EUAS

Short Biography

(i) Professional Preparation

Shandong University, Medical School	*Clinical Medicine*	*M.D.*	*1983*
Karolinska Institute, Stockholm, Sweden	*Medical Science*	*Ph.D.*	*1993*
Harvard Medical School	*Medical Research*	*Postdoc*	*1993-6*
Copenhagen University	*Medicine*	*hM.D.*	*2006*

(ii) Current and past appointments

2004-	*Professor of vascular biology, Karolinska Institutet, Stockholm, Sweden*
2010-	*Guest Professor, Linköping University, Linköping, Sweden*
2010-	*Distinguished Professor award, Karolinska Institute, Sweden*
2013-	*Guest Professor, Leicester University, Leicester, UK*
2014-	*Honorary Professor, Copenhagen University, Denmark*
2001-2004	*Associate Professor, Karolinska Institutet, Stockholm, Sweden*
2001	*Lectureship, Swedish Research Council, Stockholm, Sweden*
1998-2001	*Assistant Professor, Karolinska Institutet, Stockholm, Sweden*
1996-1998	*Senior Research Associate, Karolinska Institute, Stockholm, Sweden*
1993-1996	*Research Fellow and Instructor, Department of Surgery and Cellular Biology, Harvard Medical School, Children's Hospital, Boston, Massachusetts, USA.*
1993	*Postdoctoral Research Fellow, Ludwig Institute for Cancer Research, Stockholm, Sweden.*

(iii) Commissions of Trust and Leadership

Leadership: Board of Directors of Cancer Research at MTC, Karolinska Institute; Board Member of Management Group MTC (2004-2008); Karolinska Institute; Director of Ph.D. education in tumor biology; Chair for MTC seminars; Member of research steering group, Karolinska Institute (2000-2005); Director of Ph.D. student examinations in tumor biology MTC, Karolinska Institute; member of the board of director of Clanotech; President of the Cancer Society in Dalian; Advisor for the Acuity Pharmaceuticals.

(iv) Scientific Committees and Grant Review

*Center for Anatomie and Cell Biology, Medical University of Vienna, Austria; INSERM, France; CNR, Italy; Medical Research Council, UK; German Research Foundation, Germany; AIRC, Italy; ERC-starting grant panel member Belgium; Netherlands Organisation for Scientific Research, Netherlands; FNRSFNR, Belgium; INCA, France Institute for Basic Science (IBS), Korea; Swiss National Science Foundation, Switzerland; Canada Research Chair Program, Canada; Austrian Biological and Medical Sciences, Austria; The Belgium Research Foundation-Flanders (Fonds Wetenschappelijk Onderzoek - Vlaanderen, FWO, Belgium; Chinese Natural Science Foundation; Israel Science Foundation, Israel; Singapore Biomedical Research Council, A*STAR, Singapore; New Zealand Research Council; Irish Science Foundation; Irish Children´s Cancer Foundation; Russian Science Foundation; and the Eistein Science Foundation (Berlin) Germany.*

(v) Research monographs

Angiogenesis in Adipose Tissue. Yihai Cao, Editor, Springer. ISBN 978-1-4614-8069-3; ISBN 978-1-4614-8069-3 8eBook).

(vi) Awards and Prizes

The Dr. Axel Hirsch Prize for medicine; NOVO Nordisk Advanced grant award; European Research Council Advanced (ERC-Ad) research grant award; Distinguished professor award (Karolinska Institute); Outstanding scientist at the Karolinska Institute assessed by international panel experts;

Guest Professor, Shinshu University, Japan; Adjunct Professor at the Leicester University, UK; Guest Professor, Linköping University, Sweden; Guest Professor, Peking University, China; Honorary M.D., Copenhagen University, Denmark; Eric Fernström Prize 2003; Human Frontier Science Program (France) grant award; Human Frontier Science Program fellow; Fulbright research fellow award (USA); and Honorary professor, Copenhagen University, Denmark 2014; Chang Jiang Scholar, Chinese Educational Ministry, China; Outstanding oversea young investigator, Chinese National Foundation, China; Fellow of Thousand Talents Program, China.

(vii) Membership

Member of the EU Academy of Sciences
Member of the European Academy of Sciences and Arts
Member of American Association of Cancer Research
Member of European Foundation of the Study of Diabetes
Member of New York Science Academy

Scientific Achievements

Yihai Cao is an international leading scientist in vascular biology. Cao, born in Shandong, China, received his medical training at the Medical School, Shandong University in 1983. 1983-1986, he received further basic and clinical training from the Chinese Academy of Medical Sciences and from the Ludwig Institute for Cancer Research, Switzerland. He obtained his Ph.D. degree in 1993 from the Karolinska Institutet, followed by a 3-yr postdoctoral training period at the Harvard Medical School, Children's Hospital (Dr. Judah Folkman's Laboratory), Boston, Massachusetts. He returned to the Karolinska Institutet in 1996 and became a full professor in 2004. He received an honorary medical degree (M.D.) from Copenhagen University, Denmark in 2006. His scientific originality has led to establish a new research field of controlling metabolic diseases by targeting angiogenesis. Cao will continue to do groundbreaking research and will lead the field of angiogenesis research. He is currently a guest professor at the Linköping University, Sweden. He has recently been appointed as an honorary professor at the Leicester University, UK; and becomes an honorary professor at the Copenhagen University, Denmark. He is also honored a professorship at the Shinshu University Japan. He received the Fernström research prize in 2004. He also receives the Axel Hirsch Prize in medicine 2014. In 2010, Dr. Cao received a distinguished professor award at the Karolinska Institutet. Dr. Cao also received the ERC-advanced research grant award for being the top scientist in Europe. He received an NOVO Nordisk-advanced grant award in 2014. His research interests include molecular mechanisms of pathological angiogenesis that contributes to obesity, metabolic diseases, diabetic complications, cancer, metastasis, and cardiovascular diseases, with emphasis on clinical relevance and translational research. According to the Google Scholar Citation report, his scientific publications have been cited for 29643 times and with an h-index of 81.

In 2004, Dr. Cao´s group was one of the first in the World that described the role of angiogenesis in contribution of obesity development (**Circulation Res**, 2004). In both genetic and high fat-diet-induced mouse obese models, Dr.Cao group shows that angiogenesis inhibitors are able to inhibit and prevent obese development. These initial and groundbreaking findings have grounded the entire field of adipose vascular biology. His group then discovered several angiogenic factors in the adipose tissues that promote angiogenesis under physiological conditions. For example, they have found that leptin is a potent angiogenic factor that in collaboration with VEGF and other classical angiogenic factors including FGF and HGF promotes adipose angiogenesis (**Proc Natl Acad Sci USA.** 2001 May 22;98(11):6390-5.). They also discovered that another adipokine-adiponectin as first endogenous angiogenesis inhibitor in the adipose tissue (**Proc Natl Acad Sci USA.** 2004 Feb 24;101(8):2476-81.).

These groundbreaking findings demonstrate that adipose tissues express both pro-angiogenic and antiangiogenic factors under physiological conditions.

Based on his groundbreaking discoveries and the initial founder of the field, The Journal of Clinical investigation invited Dr. Cao to write the first autholritative review article on the topic of angiogenesis in adipose tissues and obesity (**J Clin Invest.** 2007 Sep;117(9):2362-8.). Publication of this review article in JCI has boosted tremendous interests for other scientists to work in this new field. This article has been cited for 177 times by other scientists. His group has further proceeded to use genetical models to study the role of angiogenesis in adipose angiogenesis and to reveal their functional impacts. In a FOXC2 mouse model in collaboration with Dr. Sven Enerback's group, Dr. Cao team found that FOXC2 targets the Ang2 promoter to regulate adipose angiogenesis. Exclusive expression of FOXC2 in adipose tissues resulted in hypervascularization and functional alterations of adipocytes (**Proc Natl Acad Sci USA.** 2008 Jul 22;105(29):10167-72.). Interestingly, inhibition of Ang-2 could completely block adipose angiogenesis and reverse the adipocyte functions.

Dr. Cao had the creative idea to study the role of angiogenesis in regulation of adipocyte functions. Their initial idea in this field was to use angiogenesis inhibitors for treatment of obese and diabetic animals. They treated obese and diabetic mice with an angiogenesis inhibitor TNP-470 and discovered that this angiogenesis inhibitor was able to reduce body weight and to improve insulin sensitivity without affecting food intake (**Circ Res.** 2004 Jun 25;94(12):1579-88). This is one of the first publications showing the modulation of adipose angiogenesis might offer a new therapeutic approach for treatment of obesity and type 2 diabetes. They take the advantage of cold-exposure-induced browning phenotype in subcutaneous white adipose tissues and that brown adipose tissue contain extremely high microvessel density to that the angiogenic switch and angiogenesis in regulation of metabolism. By exposing mice to cold temperature, the browning of white fat leads to a marked switch of angiogenic phenotype (**Cell Metab.** 2009 Jan 7;9(1):99-109.). They further discovered that cold-induced sympathetic activation is involved in regulation of VEGF expression in the adipose tissue, which contributes to stimulation of angiogenesis. Importantly, pharmacological inhibition of the VEGF-VEGFR2 signaling pathway completely ablates cold-induced adipose angiogenesis. Moreover, inhibition of VEGFR2 but not VEGFR1 signaling markedly inhibits non-shivering thermogenesis related to browning of the white adipose tissue. These findings demonstrate that VEGF-triggered angiogenesis is crucial for regulation of global metabolism. Thus, modulation of angiogenesis in the adipose tissue would offer a new therapeutic option for treatment of metabolic disease. In 2010, Dr. Cao was invited by **Nature Reviews Drug Discovery** (2010 Feb;9(2):107-15.) to write an authoritative review article on angiogenesis in modulation of obesity and metabolic disease. In this article, Dr. Cao proposed that stimulation of angiogenesis in white and brown adipose tissues may produce opposing effects in obesity development. This article has been cited 87 times by other scientists.

During their studies, Dr. Cao´s group has developed many unique assays in the field to study adipose angiogenesis in both brown and white adipose tissues. They have been invited to publish their methods in Nature Protocols (**Nat Protoc**. 2010 May;5(5):912-20.; **Nat Protoc.** 2012 Mar 1;7(3):606-15.). These methodologies are now widely used by others in the fields and for those who have just started to work in this interesting field. With these available methodologies and systems, Dr. Cao further discovered that a new mechanism to understand the low-temperature-related high incidence of cardiovascular diseases. By exposing ApoE-/- mice to cold, they found that cold marked augments atherosclerotic plaque development in these mice. Under this condition the plasma levels of LDL remnants are unusually high. The mechanism underlying high levels of LDL is because browning of white fat and activation of

brown fat, leading to lipolysis and cholesterol synthesis **Cell Metab.** 2013 Jul 2;18(1):118-29). This study has offered a new mechanism to explain the phenomenon of high incidence of cardiovascular disease in the cold seasons compared to warm seasons. This groundbreaking discovery received tremendous public interests including broadcasting in the hectic evening news in Swedish national TV. Very recently, Dr. Cao group has discovered that endothelial cells in angiogenic vessels produce novel angiogenic factors that could modulate adipocyte functions via a paracrine mechanism. Interestingly, blocking VEGF-medicated angiogenic factors could completely block adipocyte-mediated thermogenesis-related metabolism. Dr. Cao has been invited by the editor in Cell Metabolism to write an authoritative review article on angiogenesis in metabolism and insulin sensitivity (**Cell Metabolism**, 2013 Oct 1;18(4):478-89). Dr. Cao also served the editor for the first book (Angiogenesis in Adipose Tissue, Springer, 2013). They also discovered a novel method to switch the harmful visceral fat into beneficial energy combustion and improvement of metabolic dysfunction (**JCI Insight.** 2017 Feb 23;2(4):e89044.). They provide the first evidence that visceral fat can become brown-like adipose tissue under a physiological condition and visceral fat can be beneficial for treatment of obesity and type 2 diabetes. Additionally, they have found a new regulatory loop of browning white adipose tissue in which the stromal vascular cells control the entire adipose tissue functions via autocrine and paracrine mechanisms (**Nature Communications.** 2017 Dec 12;8(1):2079.) This groundbreaking discovery provides novel mechanistic insights on browning white adipose tissue and paves a novel avenue for potential treatment of obesity and metabolic diseases. They have developed a potential new drug for treatment of obesity and diabetes by targeting the adipose vasculature (**J Exp Med.** 2018 Jan 5. pii: jem.20171012.).

Based on Dr. Cao´s original concept and groundbreaking discoveries, the field of adipose vascular biology is now becoming emerging field of research. This field will offer new therapeutic possibilities for effective treatment of obesity and metabolic diseases including type 2 diabetes.

Cao is an internationally pioneered renown scientist in cancer research. While working with Dr. Judah Folkman, Dr. Cao was one of the team members that discovered Angiostatin (**Cell**, 1994) and showed tumor dormancy upon suppression of angiogenesis (**JCI**, 1997). He discovered several novel angiogenesis regulators including kringle proteins, chemokines and placenta growth factor-3. He also discovered one of the first oral angiogenesis inhibitor from green tea, EGCG (**Nature**, 1999). Based on his scientific findings, Dr. Cao proposed new mechanisms by which antiangiogenic therapy produces beneficial effects in cancer patients. These include off-tumor target effect (**PNAS**, 2008, **Nat Rev Clin Onco**, 2010) and reducing chemotoxicity (**PNAS,** 2010). He has made seminal contributions in understanding the complex interplay between various cellular components in the tumor microenvironment (**Nature Medicine**, 2003, **Cancer Cell,** 2002, **JCI,** 2007 and **Nature Medicine,** 2011, **Nature Communications,** 2013; **Nature Communications** under revision, 2014; **Science** 2013). He discovered several novel lymphangiogenic factors that promote cancer metastasis via the lymphatic system (**Cancer Cell**, 2004, **PNAS** 2005, **Blood** 2006). Dr. Cao was also one of the first who showed that angiogenic factor FGF could functionally recover spinal cord injury in paraplegic rats (**Science**, 1996). He also significantly contributed to development of a new technology of targeting drugs to specific tissue (**Science**, 2013). In summary, Cao is an active, imaginative, creative and dedicated scientist, who is performing groundbreaking research, educating young scientists, and spreading scientific information to the public. He is an international leading, recognized and accomplished scientist. It is very likely that his groundbreaking discoveries will lead to development of new drugs that will be used for treatment of common human diseases and save millions of lives.

Recent Developments in Materials Science of Metastable Materials

by Jürgen Eckert, Member EUAS

Short Biography

Jürgen Eckert received his Ph.D. (German: Dr.-Ing.) in Materials Science from the Friedrich-Alexander-University Erlangen-Nürnberg, Germany in 1990. During this collaborative research work with the Siemens Research Laboratories in Erlangen, he got already in touch with the topic formation of amorphous and quasicrystalline alloys through interdiffusion which he subsequently extended during his two and a half years postdoctoral stay at the California Institute of Technology („CalTech") in Pasadena, USA. There he worked with Prof. William L. Johnson on the formation of nanocrystalline alloys via high energy ball milling (mechanical alloying). After a short break in industry he moved to the Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, one of the leading Materials Research Science Centers in Germany, to continue his academic career. From 1996 till 2003 he was the Head of the Department "Metastable and Nanostructured Materials" at IFW Dresden, before he became Full Professor for "Physical Metallurgy" at TU Darmstadt, Germany. In 2006 he moved back to Dresden and was appointed Director of the Institute for Complex Materials at the IFW Dresden, and concurrently held the Chair for "Synthesis and Analysis of Materials" at Dresden University of Technology (TU) Dresden. In 2013/2014 he served as the Scientific Director of IFW Dresden, before he then moved to Austria in 2015. Jürgen Eckert currently holds the Chair "Materials Physics", serves as Head of the Department Materials Physics at Montanuniversität Leoben, and is the Director of the Erich Schmid Institute of Materials Science of the Austrian Academy of Sciences in Leoben, Austria. He also held an Adjunct Professor Position at Michigan Technological University, Houghton, USA between 2002 and 2005, and was a Visiting Professor at University of Vienna, Austria at the Institute of Physics, Physics of Nanostructured Materials (2009 / 2010 / 2012).

Jürgen Eckert was honored as Dr. honoris causa (Dr. h.c.) by the Slovak University of Technology in Bratislava, Slovak Republic (2012), and received the prestigious Gottfried Wilhelm Leibniz Award of the German Research Foundation (2009), the highest Science Prize and scientific honor in Germany. He was elected as Scientific Member of Section D of the Leibniz-Association in 2009. Other honors include the DGM-Prize 2014 of the German Materials Research Society (Deutsche Gesellschaft für Materialkunde DGM), an ERC-Advanced Grant of the European Research Council (2013), the ISMANAM Senior Scientist Award (2012), the Hsun Lee Lecture Award of the Chinese Academy of Sciences (2006), the Georg-Sachs-Prize of the German Materials Research Society and the Austrian Metal Industry (1997), and the FEMS Materials Science and Technology Prize of the Federation of European Materials Science Societies (FEMS) in 1997. In addition, he received the Young Scientist Award of the German Materials Research Society (1994), and the ISMANAM Young Scientist Award (1997).

He is a corresponding Member of the Section Mathematics-Natural Sciences of the Austrian Academy of Sciences ("korrespondierendes Mitglied im Inland") (2017), a Member of the EU Academy of Sciences (2018) and has been elected to the class of 2018 MRS Fellows of the Materials Research Society, USA (2018).

His publications have been cited more than 25.000 times and his current h-factor is 69.

Over the years, Jürgen Eckert and his team pursued research on metastable advanced high performance materials, including amorphous, nanostructured and quasicrystalline materials, and provided seminal contributions to the development and property characterization of (bulk) metallic glasses, metallic glass composites and nanostructured metallic alloys for functional and structural applications. This includes: studies on phase formation, processing and structure-property correlations of metastable materials processed under non-equilibrium conditions; processing of materials by mechanical alloying/milling; structural and functional materials and metal matrix composites with particular emphasis on solidification fundamentals; rapid solidification processing; biocompatible, magnetic and superconducting materials, and materials for energy applications and energy harvesting (e.g. next generation batteries, supercapacitors, carbon materials, materials for hydrogen storage); solidification of metal matrix composites; mechanical and electrochemical properties of bulk materials, coatings and surfaces; mathematical modelling of advanced materials and processes.

The first area of metastable phase formation concerns the synthesis of novel metastable materials through solid state reactions as can be realized through low temperature interdiffusion in nanoscale systems or through mechanical attrition involving severe plastic deformation in powders or bulk samples. Due to metastable thermodynamics and kinetic constraints combined with plasticity effects under heavily constrained conditions such processing routes allow reducing the crystallite size of solids down to the nanometer regime thus introducing a large volume fraction of interfaces. The obtained nanostructured materials can easily undergo non-equilibrium phase transformations leading to metastable phases and structures that cannot be achieved by conventional processing techniques. Examples for such metastable phases are amorphous or quasicrystalline solids with unique physical, chemical and mechanical properties that are not only of scientific interest but also turned out to be attractive for technological application, e.g. as high strength materials or for biomedical or energy applications. Along this line, also nanocrystalline or nanostructured materials can be synthesized, contributing to the ever growing field of nanostructured materials, its scientific significance and also application of nanocrystalline materials in different fields. Nowadays, nanocrystalline or nanostructured materials are one of the most rapidly growing areas of Materials Science and the number of products based on nanostructured materials is well beyond 2 billion US$ with growth rates beyond about 20% every year worldwide.

Another area of activities pursued by Jürgen Eckert and his group concerns the development and characterization of (Zr-, Ti-, Al-, Fe-, Mg-base) metallic glasses (to mention a few) and composites through non-equilibrium solidification of metallic liquids in bulk form or through condensation from the gas phase in case of thin film systems. Due to the absence of long-range translational symmetry or grain boundaries, as characteristic for (polycrystalline) crystalline solids, the amorphous structure of metallic glasses offers several advantages like enhanced strength, exceptionally large elastic limit, outstanding soft magnetic properties, high wear resistance or improved corrosion performance etc. Moreover, the occurrence of a glass transition from the amorphous solid into a supercooled liquid state opens new perspectives for the shaping of metals like plastics or inorganic glasses at high temperatures. It enables easy and cost effective production of complex-shaped parts with intricate geometry and outstanding surface quality with surface roughness on the nanometer level that can be used in net-shaped precision devices and systems. In addition, metallic glasses form for a wide range of compositions, thus

circumventing the often quite narrow composition ranges of crystalline phases. This allows varying their properties in a wide range, and fine-tuning of composition and structure provides a huge playground for adjusting materials properties like, for example, plasticity, magnetic properties, biocompatibility or catalytic performance that are technologically attractive.

In this area, the work focuses on developing plastically deformable bulk metallic glasses and composites through a synergistic approach tracking down atomic scale structures, microstructural features and stress/strain as well as processing-induced heterogeneities that determine the mechanisms of plastic deformation on different length scales to overcome the otherwise unavoidable brittleness of glassy materials. This work stretches also into areas beyond metallic glasses creating innovative strategies for the design, synthesis and characterization of intrinsic length-scale modulation and phase transformations under highly non-equilibrium conditions. This concept allows to define new routes for creation of tailored nanostructured or ultrafine-grained structural and functional materials based on scale-bridging intelligent hybrid structures enabling property as well as function optimization. Accordingly, this research spreads into the areas of materials for high-strength lightweight applications, hard and soft magnetic materials, porous bulk materials and hybrid structures for biomedical applications, materials for energy applications (metals, oxides, hierarchical carbon structures), and also touches surface modification and development of architected gradient structures. Altogether, research on metastable materials in these areas is not just driven by scientific curiosity, but also bridges the gap from fundamental research towards potential applications and use of knowledge in industry for tackling urgent needs of society in areas like for example, renewable energy systems, medical applications, development of energy efficient lightweight transportation systems, or nanostructured materials for use in devise for information technology, etc.

A third field of present activities concerns the development and application of methods for in-depth *in situ* and *in operando* investigation of phase transformations and structure-property correlations using local probes and high resolution techniques for structure characterization and imaging of local structures, chemical compositions and interaction of nanoscale objects with external fields and stimuli (e.g. mechanical, thermal, electrical, magnetic fields). Traditional Materials Science just creates novel materials systems by changing processing routes. Their properties and microstructures are analyzed, and the property-structure relationship is obtained indirectly. The vision is to overcome this paradigm by creating and testing tailored materials *in situ*, for example in a microscope. This allows controlling the desired material structure and additionally enables the direct observation of the effect of the structures on the physical or mechanical properties. An example for such an attempt is the *in situ* design and testing of metallic glass composites. As mentioned above, metallic glasses have outstanding mechanical properties and can be easily shaped, making them ideal materials for high-performance applications. Still, their low ductility at room-temperature has inhibited broad commercialization so far. This problem can be overcome by using composites of a metallic glass matrix with crystalline secondary phases, e.g. by using different external stimuli to introduce nanoscale heterogeneities into the glass. These stimuli can be a heat source or a laser, an ion or electron beam. To study the deformation at the nanoscale, *in situ* tests are carried out within a transmission electron microscope. The concept of *in situ* design and testing is applicable to a wide range of materials and is therefore expected to open a new research avenue for creating materials by design for on demand applications.

The long range perspective of these approaches and experiments is to utilize the knowledge gained in metastable materials for further advancing the understanding of structure-property correlations for hierarchically modulated structures and hybrid systems through tailoring structure formation and property optimization over a variety of different length-scales under highly non-equilibrium thermodynamic and kinetic conditions. Goal is to gain a descriptive and quantitative picture of phase formation, transformation, dynamics and property design under extreme conditions, such as ultra-fast heating and cooling on extremely short time scales with or without external mechanical, electrical or magnetic stimulus. This promises to open new avenues for nanoscale structure formation in architected materials with unique functionality. For this purpose, state-of-the-art techniques from the fields of materials physics, structure analysis, *in situ* structure investigations under different applied fields (e.g. mechanical, electrical, magnetic), and also structure-biological mimetic techniques and generative manufacturing will be used such as to generate an atomic structural – functional understanding of the properties, performance and correlation of hierarchical thin film structures and membranes, tailored interface structures, nano- and multiscale hybrid systems and tailored "lattice materials". This will also elucidate how far commonly used well-known concepts derived for micro-scale materials with varying intrinsic properties and modulated geometry can be transferred to the nanoscale. But not only the basic fundamental mechanisms of structure formation and property development will be of interest, but also the question how the findings can be transferred into parts, devices and systems for MEMS/NEMS, sensor and actuator applications, 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 tailored and personalized orthopedic implants or for advanced personalized medical devices. Altogether, this approach attempts to clarify basic questions of Materials Physics: how can one tailor architected high performance materials with exceptional properties and function through innovative materials, concepts and structure design. A detailed understanding of these questions will have implications for cross-linking Materials Science with other branches of science and possible applications in transportation, infrastructure, energy, safety, health, life sciences and information technology, and will thus contribute to tackle vital questions relevant in modern society – not only in terms of basic science, but also with respect to education of the next generation of young scientists and engineers through disseminating the findings into teaching and public outreach.

Machine Learning and Optimization for Material Design Innovation

by Timon Rabczuk

Short Biography
Prof. Dr.-Ing. at Bauhaus University Weimar, Chair of Computational Mechanics
Former Director of the Institute of Structural Mechanics, Bauhaus University Weimar
National High End Foreign Expert at Tongji University, Shanghai, China
More than 200 SCI publications
Listed in ISI Highly Cited 2014 and 2015 in 'Computer Science' and 'Engineering'
ERC-CoG COMBAT
Coordinator of ITN-INSIST and IRSES-MULTIFRAC

The design of advanced materials has become dramatically faster through using materials informatics, which provides scalable approaches to identify patterns within big data sets. Among all, materials data mining (MDM) and materials machine learning (MML) approaches have been receiving increasing attention and have achieved great improvements in terms of efficiency, robustness and prediction accuracy. Machine learning, in particular, have recently turned into a popular and powerful tool for use in materials innovation and discovery, and is playing an important role in the advancement of the materials informatics realm. To accelerate the materials design innovation, both quantitative and qualitative methods in machine learning have been adopted for different tasks in materials design, and optimization, as demonstrated in the literature. However, they found to be better suited for materials property prediction and multi-objective optimization of properties within the known range of accessible materials behavior considering the pre-existing big data sets of high dimensionality. A major challenge however would be the hierarchical nature inherent to all materials. Accordingly, to understand a material property on a given length and time scale it is crucial to optimize and predict the mechanisms on shorter length and time scales all the way down to the most fundamental mechanisms describing the chemical bond. Consequently, the materials systems are to be simultaneously studied under consideration of underlying nano-structures and meso/macro manufacturing scales. Such design process is highly nonlinear and requires an interactive design toolset. Here we describe a novel implementation of machine learning coupled with intelligent optimization to model the fundamental properties and behavior of a wide range of multi-scale materials design problems.

Machine Learning for Materials Design

The research on materials design innovation is crucial for the long-lasting success of any technological sector and industry and it is a rapidly evolving field of challenges and opportunities aiming at development and application of multi-scale methods to simulate, predict and select innovative materials with high accuracy. As reviewed by Mosavi et al.

(2018), from the development of concrete for civil constructions, to the latest innovations in lithium-ion batteries, machine learning has brought promising advancements in revolutionizing the simulation technologies and materials prediction. Machine learning is enhancing human capabilities in predicting the properties of materials. Machine learning and big data applications can perfectly use big data sets of materials and their properties to "learn" and "predict" new materials with desirable traits. Furthermore, the potential of machine learning by identifying non-linear correlations between temperature and composition and mechanical properties in nanocomposites is well stablished. In solar energy and photovoltaic sector, we can expect extraordinary with the exceptional prediction power of the data-driven modeling capability of machine learning. In medicine big data and machine learning have shown great potential in diagnostics. Thank to machine learning and the novel big data technologies the quality of microstructural image data has been highly improved, where image-driven machine learning used for microstructure prediction. As the beneficial of machine learning and data-driven modeling in materials design and computational mechanics are increasingly reported, the new frontier in materials prediction, has become also of particular interest for innovative custom-made materials. Recently, machine learning has been used in a number of cases in order to predict the fracture toughness and also to optimally design sandwich structures. We see a great potential in big data and machine learning in materials design as a new paradigm for designing materials according to their target applications. And in fact, today, the usage of big data technologies and machine learning has well stablished as a powerful computing tool for the case studies in computational mechanics which shows promising results.

Interdisciplinary Research

Thermodynamic, mechanical, and electrical structure calculations of materials, systematic storage of the information in database repositories, materials characterization and selection, and gaining new physical and environmental insights account for big data technologies. In addition, making decision for the optimal materials design needs multi-objective optimization tools as well as an efficient decision-support system for post-processing. This is considered as a design optimization process of the microstructure of materials with respect to desired properties and meso/macro functionalities. Such process requires a smart agent which learns from dataset and makes optimal decisions. The solution of this inverse problem with the support of the virtual test laboratories and knowledge-based design would be the foundation of tailor-made molecules and materials toolbox. With such an integrated toolbox at hand the virtual testing concept and application is realized. This challenging task can only be accomplished through a variety of scale bridging methods which requires machine learning and optimization combined. Furthermore a great deal of understanding on big data and prediction technologies for microstructure behavior of existing materials, as well as the ability to test the behavior of new materials at the atomic, microscopic and mesoscopic scale is desired to confidently modifying the materials properties. Numerical analysis further allows efficient experiments with entirely new materials and molecules. Basic machine learning technologies such as artificial neural networks, and genetic algorithms, Bayesian probabilities and machine learning, data mining of spectral decompositions, refinement and optimization by cluster expansion, structure map analysis and neural networks, and support vector machines, have

been recently used for this purpose.

Challenges and Research Gap

Computational materials design innovation to perfect needs to dramatically improve and put crucial components in place. To be precise, data mining, efficient codes, big data technologies, advanced machine learning techniques, intelligent and interactive optimization, open and distributed networks of repositories, fast and effective descriptors, and strategies to transfer knowledge to practical implementations are the research gaps to be addressed. In fact, the current solvers rely only on a single algorithm and address limited scales of the design problems. In addition, there is a lack of reliable visualization tools to better involve engineers into the design loop. The absence of robust design systems, lack of the post-processing tool for multicriteria decision-making, lack of Big data tools for an effective consideration of huge materials database are further research gaps reported in the literature. To conclude, the process of computational material design innovation requires a set of up-to-date solvers to cover a wide range of problems. Furthermore, an advanced database would require cloud computing, big data technologies, learning from data and a powerful set of intelligent optimization tools. The other problems with current open-source software toolboxes, is that they require a concrete specification on the mathematical model and also the modeling solution is not flexible and adaptive. This has been a reason why the traditional computation tools for materials design have not been realistic and as effective. Consequently, our vision is to propose an interactive toolbox, where the solver determines the optimal choices via visualization tools. Ultimately the vision is to construct a knowledge-based virtual test laboratory to simultaneously optimize the hybrid materials microstructure systems, e.g. textile composites, at atomic, microscopic, and meso/macroscopic scales. Whether building atomistic, continuum mechanics or multiscale models, the toolbox can provide a platform to rearrange the appropriate solver according to the problem at hand. Such platform contributes in the advancement of innovative materials database leading to innovative materials design with the optimal functionality.

Machine Learning Coupled with Optimization

The complex body of information of computational material design asks for the most recent advances in machine learning and optimization to scale to the big data and multi-objective nature of problems to direct prediction for an optimal design. From this perspective the materials design can be seen as a high potential research area and a continuous source of challenging problems for machine learning. The vision would be an automated system so that only data and the desired outputs need to be provided where machine learning is used for selection the multiscale 3D materials structures. Furthermore, machine learning is used to combine heterogeneous and noisy sources of information from evolutionary, similarity and experimental data in order to contribute in discovering relational structures. In the proposed approach every individual design task, according to the problem at hand, can be modeled on the basis of the solvers within the toolbox. To obtain a design model the methodology does not ask to specify a model, but it experiments with the current system. The appropriate model is created in the toolbox and further is used to identify a better solution in a learning cycle. The methodology is based on transferring data to knowledge to optimal decisions through machine learning i.e. a workflow that is referred to as prescriptive analytics. In addition, an efficient big data application can be

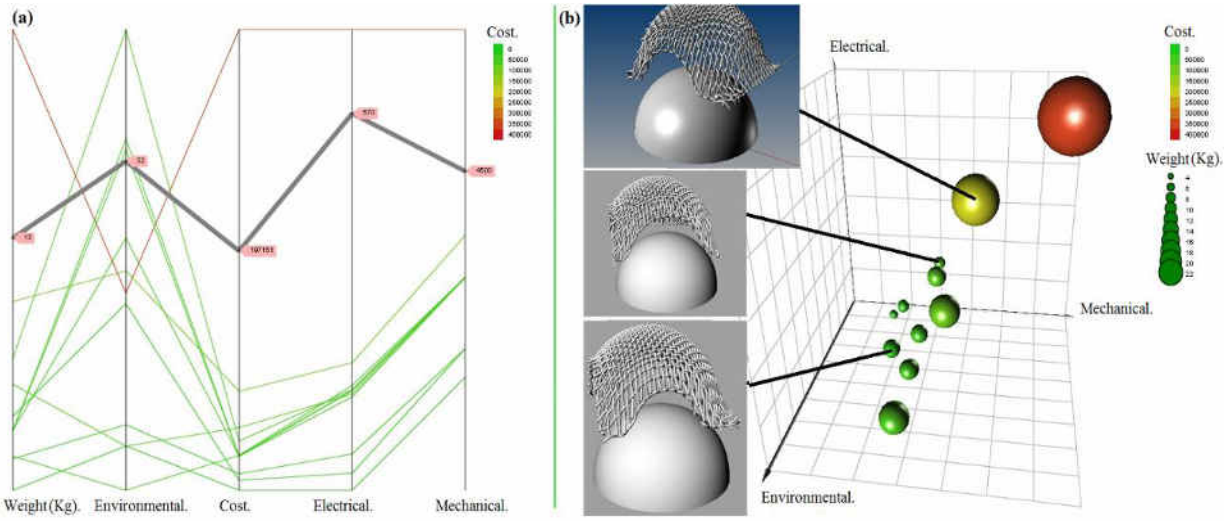
integrated to build models and extract knowledge. Consequently, a large database containing the thermodynamic and electronic properties of the existing and hypothetical materials is interrogated in the search of materials with the desired properties. Knowledge exploits to automate the discovery of improving solutions i.e. connecting insight to decisions and actions. As the result a massively parallelized multiscale materials modeling tools that expand atomistic-simulation-based predictive capability is established which leads to rational design of a variety of innovative materials and applications.

A variety of solvers integrated within the proposed solver include several algorithms for data mining, machine learning, and predictive analytics which are tuned by cross-validation. These solvers provide the ability of learning from data, and are empowered by reactive search optimization (RSO) i.e. the intelligent optimization tool that is integrated into the solver. The RSO fosters research and development for intelligent optimization and Reactive Search. Reactive Search advocates the integration of sub-symbolic machine learning techniques into local search heuristics for solving complex optimization problems. The word reactive hints at a ready response to events during the search through an internal online feedback loop for the self-tuning of critical parameters. In fact, Reactive Search is the effective building block for solving complex discrete and continuous optimization problems which can cure local minima traps. Further, cooperating RSO coordinates a collection of interacting solvers through an organized subdivision of the configuration space which is adapted in an online manner to the characteristics of the problem. Such implementation has been recently used for a number of problems e.g. material selection, engineering design, and computational mechanics.

Textile Composites Optimal Design

This case study presents a novel application of the machine learning coupled with optimization, dealing with decision conflicts often seen among design criteria in composite materials design (Mosavi & Rabczuk, 2017). In the integrated design processes of composite materials, it is necessary to explore optimal design options by simultaneously analyzing material properties in a multitude of disciplines, design objectives and scales. The complexity increases with considering the fact that the design objective functions are not mathematically available and designer must be in the loop of optimization to evaluate the meso/macro manufacturing scales of draping behavior of textile composites. This case study describes a classic textile composite design problem with a relatively large-scale decision space with the multi-disciplinary property values of electrical, mechanical, weight, cost, and environmental attributes. To solve the problem a multi-objective optimization model is required to formulate and systematically compare different alternatives against large sets of design criteria to tackle complex decision-making task of exploring trade-offs and also designing break-even points.

The integration of machine learning and optimization can be customized for different problems and usage contexts in material design. In this case study the Grapheur is used to provide an interactive optimization toolset highly suitable for the problem at hand. Interactive multi-objective optimization of Grapheur has a strong user interface for visualizing the results, facilitating the solution analysis, decision-making process, and post-processing. With the decision maker in the loop, effective interactive schemes are developed where it provides a versatile tool for stochastic local search optimization.



Interactive multi-objective optimization toolset: exploring trade-offs and break-even points: parallel chart considering five objectives (a) 7D visualization graph for post-processing: simultaneous screening the meso/macro manufacturing scales (b).

Conclusions

Computational material design innovation is an emerging area of materials science aiming at development of multiscale methods to predict, select, and simulate innovative materials. Yet it requires an adaptive solver to rule a wide range of materials design problems. We provide a suitable platform for developing a computational toolbox for the virtual design and simulation-based optimization of advanced materials to model, simulate, and predict the fundamental properties and behavior of multiscale materials. The proposed solver is a simple yet powerful concept presenting an integration of advanced machine learning and intelligent optimization techniques. With a strong interdisciplinary background, the novel application connects computer science and engineering, and further strengthens the research direction of digital engineering.

Acknowledgements
This article was written in cooperation with Dr. A.Mosavi.

Bibliography

Mosavi A., Rabczuk T., Varkonyi-Koczy A.R. (2018) Reviewing the Novel Machine Learning Tools for Materials Design. Recent Advances in Technology Research and Education. pp 50-58, vol 660. Springer.

Mosavi A., Rabczuk T. (2017) Learning and Intelligent Optimization for Material Design Innovation. Learning and Intelligent Optimization. pp 358-363. Lecture Notes in Computer Science, vol 10556. Springer, Cham

The Essence of Importance Measures

by Way Kuo, Member EUAS

Short Biography

Professor Way Kuo is President of City University of Hong Kong. Before he came to Hong Kong in 2008, he served on the senior management team at the Oak Ridge National Laboratory and as the Dean of Engineering at the University of Tennessee, Knoxville.

In addition to being a member of the US National Academy of Engineering, he is a foreign member of the Chinese Academy of Engineering, a foreign member of the Russian Academy of Engineering, and a member of Academia Sinica in Taiwan. He is a pioneer in designing and modelling the reliability of electronics systems at the infant stage, renowned for his work on designing reliability in electronics systems. He is the author and co-author of ten academic books and over 200 high impact papers, some of which are deemed classics in systems optimisation design and are used as the basis for establishing the reliability standards. His book, Importance Measures in Reliability, Risk, and Optimization, published by N.Y.: Wiley, 2012, addresses ways to design and enhance reliability of modern systems.

His first popular science book, Critical Reflections on Nuclear and Renewable Energy, has had an impact since its publication in 2013 by Commonwealth Publishing Group in Taiwan. The book has been translated into English, Japanese, French and Russian and published in Massachusetts, Tokyo, Paris, and Moscow, respectively. His new book on higher education, The Soulware with Higher Education, was simultaneously published in Hong Kong, Taipei and Beijing in 2016 under three different publishing houses.

Professor Kuo is the Chairman of the Gnedenko e-Forum based in Moscow, Russia.

A system normally consists of multiple components, which are not necessarily equally important for the performance of the system. Such a system often needs to be designed, enhanced, or maintained efficiently using limited resources. However, for highly complex systems, it may be too tedious, or not even possible, to develop a formal optimal strategy. In these situations, it is desirable to allocate resources according to how important the components are to the system and to concentrate the resources on the small subset of components that are most important to the system. Thus follows the notion of importance measures of components.

For tackling different problems, the distinct importance measures and the associated algorithms should be appropriately designed. Various importance measures have been proposed to judge the relative strength of a component in a system with respect to different criteria. As stated in Griffith and Govindarajulu (1985), no single type of importance measure is universal, since different perspectives on the same system can lead to different views about which factors make one component more important than another. A design engineer may think of a component as being more important if a given reliability improvement in it does more to improve systems reliability than the same reliability improvement in another component. In contrast, an engineer may devise a checklist of components for finding the cause of system failure based on his or her assessment of the conditional probability that a particular component has contributed to system failure. The probabilistic interpretation describing the relation of a component to the functioning or failure of the system is different in each case.

Materials and Process Modelling Technologies

by Jianguo Lin, Member EUAS

Short Biography

Name: *Professor Jianguo Lin FREng, PhD, CEng, FIMechE, FIMMM*
Date of Birth: *18 June 1958*
Nationality: *British*

EDUCATION

1. *Xinjiang Shihezi University (March 1978 – Jan. 1982). BEng, Mech. Eng., 1982.*
2. *Taiyuan University of Technology (Feb. 1982 – Jan. 1985). MEng, Mech. Eng., 1985.*
3. *University of Sheffield (1988 - 1991). PhD, Mech. Eng., 1991.*

MEMBERSHIP OF PROFESSIONAL BODIES:

1. *Fellow of Royal Academy of Engineering (**FREng**)*
2. *Fellow of Institution of Mechanical Engineers (**FIMechE, CEng**)*
3. *Fellow of Institute of Materials, Minerals and Mining (**FIMMM**)*

CURRENT POST

- *Professor in Mechanics of Materials (April 2008 – present). TATA Steel/RAEng Research Chair. Head of Mechanics of Materials Division, responsible for various activities, including budget, labs and 4 research groups of the Division, which has some 20 academic staff and over 130 Postdoctoral Researchers and PhDs.*
- *Director of Manufacturing Future Lab. of Imperial College London (over 20 academic staff from different departments and faculties across the College).*
- *Director of BIAM Centre for materials characterisation, processing and modelling (involving 2 Departments (Mech. and Materials), 8 academic staff and about 15 researchers).*
- *Director of AVIC Centre for structural design and manufacture (involving 2 Departments (Design and Mech.), 6 Academic and 16 researchers).*
- *Founding Director (Non-executive) of Impression technologies Ltd, which is a Spin-off company of Imperial, Established in 2013 and now have over 50 employees with the world first HFQ® dedicated production line in Coventry. (HFQ® is a trade mark registered by Impression Technologies Ltd).*

PREVIOUS POSTS

- *Lecturer (1996–2004), Senior Lecturer (2004-2006), Reader in Solid Mechanics (2006-2008), Dept. of Mech. Eng., Univ. of Birmingham.*
- *Post-doctoral Research Associate, University of Sheffield, Oct. 1991- Feb. 1993; and, UMIST, Feb. 1993 - Feb. 1996.*

RESEARCH GRANTS AND CONTRACTS

Professor Lin has been successful, as a principal and co-investigator, in obtaining research grants worth a total of over £16 million, and involved projects over £70 million, from the UK government (EPSRC & DTI/TSB, Innovate-UK), European Commission, UK and overseas industries.

Selected Funded Research Projects:

2017-2022 ***J. Lin****, N. Li and J. Jiang,* ***LightForm:*** *Embedding Materials Engineering in Manufacturing with Light Alloys, (3 Partners, Let by Manchester Uni., Total Funding: £5,888,670), EP/R001715/1, EPSRC*

2018-2021 ***J. Lin,*** *B. Blackman, J. Jiang, Rapid Aluminium Cost Effective Forming (**RACE-Form**), (6 Partners, Lead by ITL, Total Funding: £9,800,000), APC 7, Innovate-UK & EPSRC*

2016-2019 ***J. Lin*** *& L. Wang,* ***LoCoMaTech*** *— Low Cost Materials Processing Technologies for Mass Production of Lightweight Vehicles****.*** *H2020-NMBP-GV-2016 (723517), (19*

partners from 9 countries, Total: €7,997,725; ICL: €1,305,092 – JL: Coordinator), EC.

2015-2020 ***J. Lin****, L. Wang, CSR Sifang–Imperial Joint Research Centre for Rail Transportation Manufacturing Technologies* ***(£2.5 Million),*** *CSR Qingdao Sifang Locomotive Vehicle Co. Ltd.*

2015-2020 ***J. Lin*** *- TATA Steel/RAEng Research Chair in Multidisciplinary studies of hot stamping,* ***£739,608*** *(TATA Steel: £471,481.75; RAEng: £268,126.89).*

2015-2018 ***J. Lin*** *and D. Balint - New aerospace advanced cost effective materials and rapid manufacturing technologies (MMTech) EC H2020 (13 partners from 4 countries; Total: €5,710,942;* ***ICL: €423,625****),*

2013-2016 ***J. Lin*** *& L. Wang & D. Balint,* ***LoCoLite*** *— An industry system enabling the use of a patented materials processing technology for Low Cost forming of Lightweight structures for transportation industries****.*** *FP7-NMP-2013-SME-7 (604240-2 LoCoLite CP-TP), (16 partners, Total: €6,083,371; ICL: €1,022,207 – JL: Coordinator), EC.*

2012-2022 ***J. Lin****, J. Dear & K Nikbin, AVIC Centre for Structural design and manufacture,* ***(£11,500,000****), Aviation Industry Cooperation of China (AVIC).*

2009-2012 ***J Lin*** *and D Balint, Warm Aluminium Forming Technology (WAFT), (Total: £2,760,000), TSB/EPSRC/Jaguar (plus 6 other UK companies).*

2008-2011 ***J Lin*** *and D Balint, Multiscale Modelling for Multilayered Surface Systems (M3-2S), EU FP7 (NMP-2007), (Total Funding* ***€4,560,000*** *Euros for 12 partners, J. Lin–Coordinated the overall project), Imperial College: 697,640 Euros. European Commission.*

2007-2010 ***J Lin****, M Strangwood and TA Dean, A novel process: solution-Heat-treatment, Forming and cold-die Quenching (HFQ),* ***£462,332****, EPSRC.*

2007-2010 P Bowen & ***J. Lin****, Process modelling for tomorrow's engines (****PROMOTE****), DTI/EPSRC/Rolls-Royce (Total: £2m, Birmingham:* ***£520,000****, lead by Rolls-Royce).*

AWARDS:

2016 "The Davey Udual Award" for his Major contribution to technical development in the sheet metal industry, Institute of Sheet Metal Engineering (ISME, UK).

2016 The President's Award for Excellence in Research, 2016. Imperial College London.

CONTRIBUTION TO INTERNATIONAL JOURNALS

A member of the ***editorial board*** *for* ***5 international journals****: (Int. J. of Machine Tools and Manufacture, Engineering Transactions, Int. J. of Damage Mechanics, Open Mechanics Journal, J. of Multiscale Modelling.)*

PUBLICATIONS

- *Author or co-author for* ***265*** *papers, of which* ***186*** *are full-length papers in refereed journals,* ***9*** *chapters in edited books,* ***73*** *papers in conference proceedings and* ***56*** *other research publications (including user manuals for testing and software systems) for companies and research collaborators.*
- ***18 filed/awarded patents****. Including: HFQ®-Aluminium technology; Multi-materials lightweight gear forging; Low-temperature press hardening for Boron steel; A combined additive manufacturing and forging technique; Flexible tooling technology for creep age forming; A method for producing curved extrusion profiles.*
- ***2 books****. One solely authored book and one edited book.*
- *Edited* ***8*** *special issues for international journals.*

EDUCATION AND TRAINING FOR "MANUFACTURING plc"

Professor Lin has developed novel teaching materials, methods and techniques for undergraduate teaching, which have been published in the *International Journal of Mechanical Engineering Education* [1]. In addition, he has educated a group of postdoctoral researchers and doctoral students in the high-value manufacturing processes

and techniques for which he has been responsible. He created a metal-forming course in 2011 at Imperial; "Metals Processing Technologies" for MEng/MSc students, dedicated to industrial needs.

RESEARCH EXPERIENCE

Professor Lin's research expertise is in Materials and Process modelling, Solid/Computational Mechanics, which includes micro-mechanics modelling, and its application in creep-damage, cyclic-plasticity, viscoplasticity and advanced materials processing technologies. He established a Metal-forming and Materials Modelling Group at Imperial College London in 2008 and this has now expanded to over 70 researchers, providing R&D services for aerospace/aeronautical, automotive, railway, metal-packaging and materials processing industries. The Group has an international reputation in the development of new metal forming processes, multiscale materials and process modelling. Significant research funding (PI: over £16 million and involved in over £70 million) has been received from EPSRC, TSB/Innovate-UK, EC, UK and overseas industries.

He led the Metal Forming Group at Birmingham University from 2001 to 2008, extending the research activities of the Group and changing the emphasis from primarily forging to materials and process modelling (including micro-mechanics modelling), prediction of microstructure evolution in warm/hot forming processes, hybrid sheet metal forming and micro-forming. His contributions to engineering science are unique within the field of computer optimisation of manufacturing technologies and processes. He has pioneered the symbiosis of classical mechanics (e.g. Ford, Johnson, Hill, etc, in 1930 - 1960s) and physical metallurgy by utilising state-variable material descriptions with calibrated multiple differential equations [2,3,4,5]. The outcome is an ability to simulate a wide range of manufacturing processes in a way that enables control of key metallurgical states to achieve the desired mechanical properties in the required locations within engineering components.

Professor Lin has pioneered these developments over recent decades and has achieved international recognition. By virtue of his scientific esteem and ability to interact with both engineers and materials scientists he was shown a unique ability to bring together groups of academics and engineers of major international manufacturing and materials processing companies to establish collaborative research projects. For examples, he has been involved in the organisation/management of an FP6 Integrated project, "Integrated Systems for Mass Production of Miniature/Micro Components – MASMICRO (FP6-IP-500095-2; Total: 21.5 Million Euros)", which include 36 partners (24 from industries) from 11 countries (2004-2008). He coordinated a project of "Multiscale Modelling for Multilayered Surface Systems – M3-2S (FP7, NMP-SL-2008-213600; Total: 4.56 Million Euros)", which includes 12 partners (7 from industries) from 7 countries (2008-2011). He coordinated "Low Cost Materials Processing Technologies for Mass Production of Lightweight Vehicles – LoCoMaTech" (H2020-NMBP-GV-2016 (723517), 19 partners from 9 countries, Total: €7,997,725). His major engineering, scientific and industrial contributions include the following aspects.

- **Proposed new theories for modelling microstructure and damage evolution in hot/warm materials processing** [2, 5, 6, 7]. The theory has been accepted by the metal forming community and used in companies for materials processing design and

optimisation. This enables materials to be processed with known microstructure and mechanical properties at the required locations.

- **Originator of Evolutionary Algorithms (EA)-based optimisation software systems for determining material models from experimental data** [8, 9]. This provides an efficient automatic means for determining material models for engineering applications. The theories and the systems have been used for solving real problems for many companies including Corus UK Ltd, Rolls-Royce, Doncasters Plc, Arcelor-Mittal (France), Israel Aircraft Industries (Israel), ESI Group.
- **Micro-mechanics modelling**. He has developed new unified crystal plasticity constitutive equations and a crystal plasticity FE process modelling system, VGRAIN (a unique system in the world), which, coupled in commercial FE codes, has been successfully used for process modelling for forming micro parts. The size effect and localised necking/failure features in micro-forming can be captured and predicted. VGRAIN (a unique system in the world) is widely used in micro-forming simulations [10].
- **Theory in Creep Age Forming (CAF**). He created a unique theory for modelling creep ageing hardening behaviour of materials in CAF. The theory has been used by ESI (a world leading software company headquartered in Paris) for their commercial FE system, PAMSPAMP, for aerospace and rail industries [6, 11].
- **New metal forming technologies.** Such as, (i) HFQ®-technology [12]. Based on the patented technology, a spin-off company, Impression Technologies Ltd, was established in 2013 and now have over 50 employees and a world first HFQ® dedicated production line established in Coventry providing high-value lightweight panel parts for Aston-Martin, Lotus, and many other automotive companies worldwide. (ii) Multi-materials lightweight gear forging technique; (iii) Low temperature hot stamping of Boron steel; (iv) Double side extrusion technology.

References

1. J. Lin and A.A. Ball, 1998, A laboratory project-based teaching approach to integrated design, *Int. J. of Mech. Eng. Education,* **26**, 318-326.
2. J. Lin, 2015, "*Fundamental of materials modelling for metal processing technologies*". World Publishing. ISBN: 978-1-78326-496-4.
3. J. Lin, F.P.E. Dunne and D.R. Hayhurst, 1996, Physically-based temperature dependence of elastic viscoplastic constitutive equations for copper between 20 and 500 ^{O}C, *Philosophical Magazine A,* **74**(2), pp655-676.
4. B.F. Dyson, D.R. Hayhurst and **J. Lin,** 1996, The ridged uniaxial testpiece: large-displacement finite element predictions of creep fracture modes, strain in homogeneities and measurement errors, *Phil. Trans. R. Soc. Lond A*, **452**, pp655-676**.**
5. J. Lin, Y. Liu, D.C.J. Farrugia and M. Zhou, 2005, Development of dislocation based-unified material model for simulating microstructure evolution in multipass hot rolling, *Philosophical Magazine A,* **85**,1967-1987.
6. J. Lin, K.C. Ho and T.A. Dean, 2006, An integrated process for modelling of precipitation hardening and springback in creep age-forming, *Int. J. of Machine Tools & Manufacture*, **46**, 1266-1270.
7. J. Lin**,** 2003, Selection of material models for predicting necking in superplastic forming, *Int. J. of Plasticity,* **19**, 469-481.
8. J. Lin and J. Yang, 1999, GA based multiple objective optimization for determining viscoplastic constitutive equations for superplastic alloys, *Int. J. of Plasticity***, 15**, 1181-1196.

9. B. Li, J. Lin and X. Yao, 2002, A novel evolutionary algorithm for determining unified creep damage constitutive equations, *Int. J. of Mech. Sci.,* **44**, 987-1002.
10. P. Zhang, M. Karimpour, D. Balint, J. Lin, D. Farrugia, 2012, A controlled Poisson Voronoi tessellation for grain and cohesive boundary generation applied to crystal plasticity analysis, *Computational Materials Science,* **64**, 84–89.
11. Y. Li, Z. Shi, J. Lin, Y-L. Yang, etc., 2017, A unified constitutive model for asymmetric tension and compression creep-ageing behaviour of naturally aged Al-Cu-Li alloy, *Int. J. of Plasticity*, **89**, 130-149 .
12. P.R. Garrett, J. Lin and T.A. Dean, 2005, An investigation of the effects of solution heat treatment on mechanical properties for AA 6xxx alloys: experimentation and modelling, *Int. J. of Plasticity,* **21**, 1640-1657.

New Aspects for Development of Green Cements and Sustainable Infrastructure

by Paulo Monteiro, Member EUAS

Short Biography

Professor Monteiro is the Roy W. Carlson Distinguished Professor at the Department of Civil and Environmental Engineering, University of California, Berkeley. He is at the forefront of developing strategies to improve the long-term performance of concrete structures. The first to develop soft X-ray spectromicroscopy using synchrotron radiation to image chemical reactions in real time, he modernized the study of hydration mechanism. Professor Monteiro's achievements in experimental research include: (1) pioneering the use of low-temperature scanning electron microscopy to image ice formation in porous cement paste; (2) developing total scattering methods to study calcium silicate hydrates in order to optimize its nanostructure; (3) creating the first high-resolution nanotomography of hydration products using X-rays; and (4) engineering a comprehensive nanostructure characterization of ancient Roman concrete to unlock the secret of its durability. His contributions also include developing rigorous mathematical theories to model material behavior, such as: analysis of interphases in concrete, modeling cryo-suction of concrete exposed to freezing temperatures using poromechanics, scaling laws for durability predictions, and fluid flow in nano-porous media. He has published over 260 archival papers and co-authored with P.K. Mehta the classical textbook, Concrete: Microstructure, Properties, and Materials, 4th edition, McGraw Hill, (2014), which has been translated to Japanese, Chinese, Greek, Spanish, Portuguese, and Persian.

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

With an estimated yearly consumption approaching 30 billion tonnes, concrete outpaces the per capita production of any other material (Fig. 1). Unfortunately, America's infrastructure was built mostly during the 1940s and is now aging and needs to be replaced. This widespread crisis threatens public safety, industrial development, and economic growth. On March 19, 2013, the American Society for Civil Engineers (ASCE) released its fifth *Report Card for America's Infrastructure*. Conducted by an Advisory Panel composed of the nation's leading civil engineers whose areas of expertise cover a broad spectrum, ASCE conferred an overall grade of "D+" and estimated that an investment of 3.6 trillion U.S. dollars will be needed to raise the grade to a "B" level by 2020.

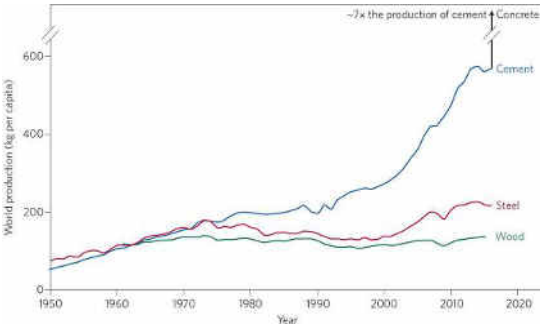


Figure 1 Historical growth in infrastructure material demand as exemplified through per capita cement, steel and wood production. Note that the production of cement correlates approximately to a mass of concrete that is seven-fold larger than that of cement alone. (Monteiro et al., *Nature Materials*, V. 16, 7, 698-699, 2017)

Portland cement is a manufactured product that is the principal hydraulic binder used in modern concrete mixtures; it is not only energy-intensive (4 GJ/tonne of cement) but also responsible for large emissions of CO_2. The manufacture of 1 tonne of PC clinker releases 0.8 to 1 tonne CO_2 into the atmosphere. The world's yearly cement production of 4.2 billion tonnes of mostly PC is responsible for nearly 7% of the total global CO_2 emissions. Little is known, however, about its water consumption as well as the effective measures to reduce such consumption. Together with Prof. Miller from UC Davis, we quantified the water use of global concrete production in 2012 and project the value to 2050. The results show that concrete production was responsible for 9% of global industrial water withdrawals in 2012 (this is approximately 1.7% of total global water withdrawal). Figure 2 shows the current and project water stress due the production of concrete.

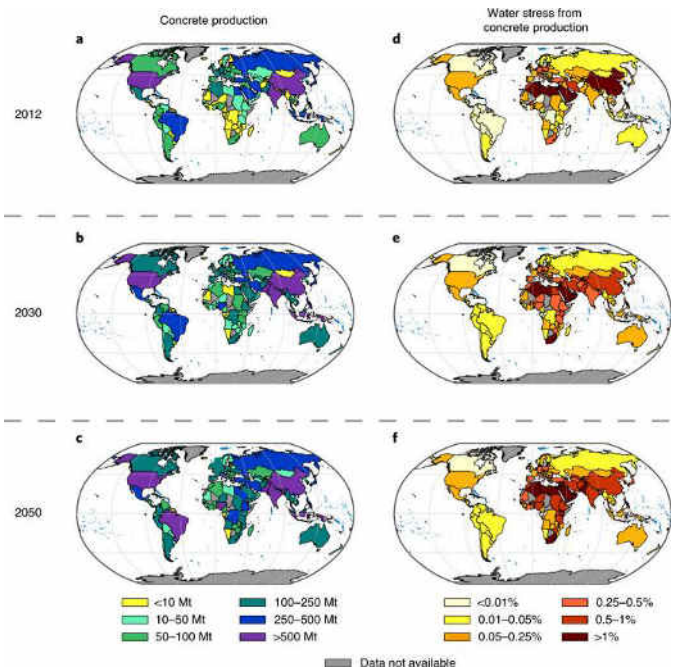


Fig. 2 Current and projected changes in water stress from concrete production relative to concrete production.
a–c: Estimations for concrete production for each country reporting production are plotted. Mt, megatonne.
d–f, Water stresses associated with concrete production for the countries with both cement production and renewable water-resource data. Water stress is shown as water withdrawals from the production of concrete relative to the available renewable water resources
Miller et al., *Nature Sustainability*, 1, 69–76, 2018.

The microstructure and properties of concrete can be altered by cost-effective methods that improve the impermeability and durability on exposure to weather extremes. At present, most of the feasible options for microstructural improvement have already been implemented. Thus, there is an urgent need to find scientific and technically-viable improvements in the atomic and nanostructure of the cementitious phases to increase concrete strength and durability. Such improvements will reduce the cement content in a concrete mixture and, therefore, its carbon footprint. Optimizing the properties of Portland cement, concrete's principal binding phase, calcium silicate hydrate (C-S-H), is a potential strategy to achieve concrete with better performance and more durability while still reducing its carbon footprint. Calcium silicate hydrate exists as a solid solution with variable structure and chemical composition, and can coexist with other solid phases at thermodynamic equilibrium. It is also poorly crystalline and hierarchically porous at

multiple length scales. Such characteristics make it exceedingly difficult to probe composition-structure-property correlations of pore-free C-S-H. Calcium aluminosilicate hydrate (C-A-S-H) can be formed when supplementary cementitious materials (SCMs), such as fly ash, blast-furnace slag, and volcanic ash, containing aluminum. Calcium aluminosilicate hydrate synthesized hydrothermally at room temperature lacks long-range crystallinity but has an atomic structure analogous to tobermorite, i.e., stacked layered structures (along the ***c***-axis), with aluminosilicate dreierketten chains clamping on either side of CaO_7 double sheets, with zeolitic water and charge-balancing ions (e.g., Ca^{2+}) in the interlayer space (see Fig. 3a). Every two-paired-site $Si(Al)O_4$ tetrahedra are connected by a bridging site tetrahedron in the dreierketten chain structure, which runs parallel to the ***b***-axis. The intralayer and interlayer, as separated by the bridging Si site, together lead to basal spacings of ~9-16 Å in the C-(A)-S-H structure, see Fig. 3b

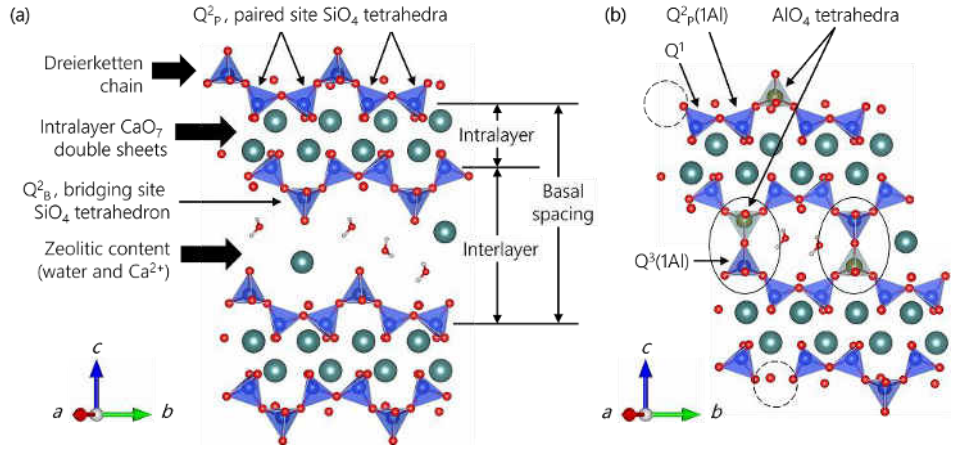


Figure 3. Schematics of (a) crystalline C-S-H (modified from 14 Å tobermorite) and (b) C-A-S-H atomic structures with Al-induced cross-linking (solid circles). Spheres of blue, red, green, white, and yellow colors represent Si, O, Ca, H and Al, respectively; and (b) the dashed circles are tetrahedral Si vacancies in bridging sites. The conventional $Q^n(m\text{Al})$-notation is used, which describes aluminosilicate chain polymerization, e.g., Si tetrahedra are connected to n adjacent tetrahedra (SiO_4 or AlO_4), of which m are AlO_4; subscripts P and B represent paired and bridging sites, respectively (after Myers *et al.*, 2015, *Cem. Concr. Res.*, 68, 83–93).

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

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

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

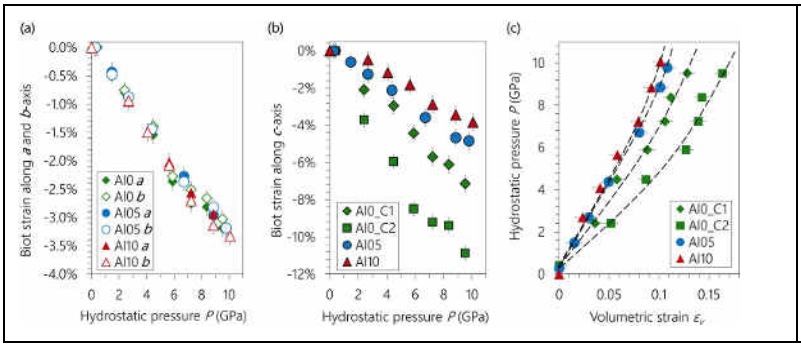


Figure 4. Biot strains as functions of applied hydrostatic pressure along (a) a- and b-axes, (b) c-axis, and (c) hydrostatic pressure as a function of volumetric strain. (Geng et al., *Scientific Reports*, 2017)

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

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

Using limited angle nano-tomography from TXM transmission images, our team obtained the first high-resolution 3D images of hydrated cement paste. Although a single 2D transmission image is not sufficient to get a 3D representation of a complex pore network, the one-frame-per-second investigation of the sample is perfectly adequate for kinetic studies. Based on the Fourier slice theorem, it is possible to compute ultra-small angle-scattering patterns; however, it remains a challenging experiment that is largely used to characterize geomaterials. The technique has become much more powerful with the advent of soft X-ray ptychography, which uses coherent diffraction patterns and allows a high spatial-resolution morphology. Our research group reported the first use of high-resolution soft X-ray ptychrography image of C-S-H and morphological quantification of C–S–H, to distinguish the contributions of C–S–H forming inside the original cement grain and the C-S-H formed in the space between grains to the small angle scattering of cement paste (see Figure 5). This line of research may provide unique information on the meso-structure of the cementitious matrix in concrete.

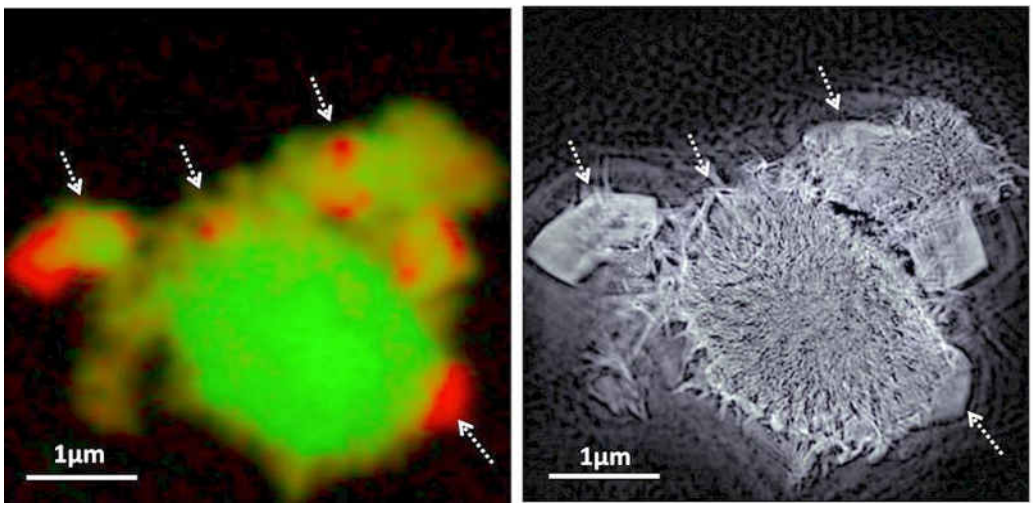


Figure 5. Traditional Scanning Transmission X-ray micrograph (left) and a soft X-ray ptychographic image (right) of 17 d hydrated cement grain. The soft X-ray ptychographic was able to image the individual fibers of C-S-H (from Bae *et al.,* 2015, *J. Am. Ceramic Soc.*, doi:10.1111/jace.13808)

Solutions for Century Old Engineering Problems

by William Gerberich

Short Biography

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

Awards

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

Extras

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

While one might cite 1754 BC as recognizing the existence of serious infrastructure problems in an organized society, most of the following is 20th century and beyond. What I mean by infrastructure is that fracture problems were endemic and highlighted in the

Code of Hammurabi [1,2] where he stated "*If a builder build a house for someone, and does not construct it properly, and the house which he built fall in and kill its owner, then that builder shall be put to death."* Fast forward to (1911) during which the Titanic failed with no similar retribution. The ship failure was attributed to be faulty steel but it was really faulty iron rivets (not the steel hull) as documented recently [3]. Future ship building eventually avoided rivets but steel ships constructed suffered as many as 1500 brittle fractures on Navy ships by about 1946. While many of those ships did not sink, a large number did and the basis for the selection of steels used was predominantly based upon the Charpy V-notch impact test, *circa 1900*. That eventually became an ASTM Standard (E28). There was little attempt to put this on an engineering and physics-based solution until the 1950s by Irwin [4], Eshelby and Bilby [5]. While this produced a flashed response of Fracture Mechanics programs between 1970 and 1990, this soon diminished with other funding pressures associated with the internet explosion and health research. For example, between 1970 and 1990, the NIH budget tripled from 10B$ to 30B$ while NSF's only increased from about 3B$ to 6B$. Since 1990 there have been a few studies but this century – old problem still does not attract adequate attention.

This submission is not a full-proof solution but is a pathway that could represent a more rigorous approach to this century old problem. In discussions with colleagues, there is an agreement that with the advances of the last two decades in computational power and powerful instrumentation diagnostics, that relatively simple algorithms based upon known physics and mechanics, could speed up material developments. Here we discuss two examples of one semiconductor and one metal to demonstrate the power of a simple algorithm being able to predict desired outcomes by changing two parameters that would be independently measureable. Since it is assumed that known chemistry, microstructure and/or processing has been or could be changed slightly to provide the known quantities needed, the outcome to improved strength-toughness combinations would evolve. While one might view this as machine learning, it is constrained by the known chemistry and processing variables already in place and as such becomes an optimization exercise.

Two examples of a brittle to ductile transition, one quite brittle being single crystal silicon, and one more ductile of tungsten are highlighted. In both of these, three key properties are needed, that of an effective shear yield stress,τ^*,and another of an activation volume,,V^*, for which the product extrapolated to zero degrees kelvin will give an activation energy for dislocation nucleation using kink pairs. The reader is referred to two publications, Hirth and Loethe,[6] and E. Hintsala,et al [7] for additional information as to what kinks are and how to measure their energy. Once one has these two parameters and H_0, the activation energy, a simple equation can be used to calculate a strain energy release rate, G_{Ic}, from which a fracture toughness may be calculated from linear elastic fracture mechanics, from

$$K_{Ic} = [E\, G_{Ic}]^{1/2} \text{ for plane stress} \qquad (1)$$

or incorporating $1/1-\upsilon^2$ in the denominator for plane strain, K_{Ic}. For silicon single crystals, a technique has been developed [4] which allows cracks to develop and arrest due to the design of a 3-pt. bend sample of 1-μm thickness. This is shown in Figure 1 and due to bend constraint, the initial FIB notch will be arrested after short extension. Details are explained elsewhere [8].

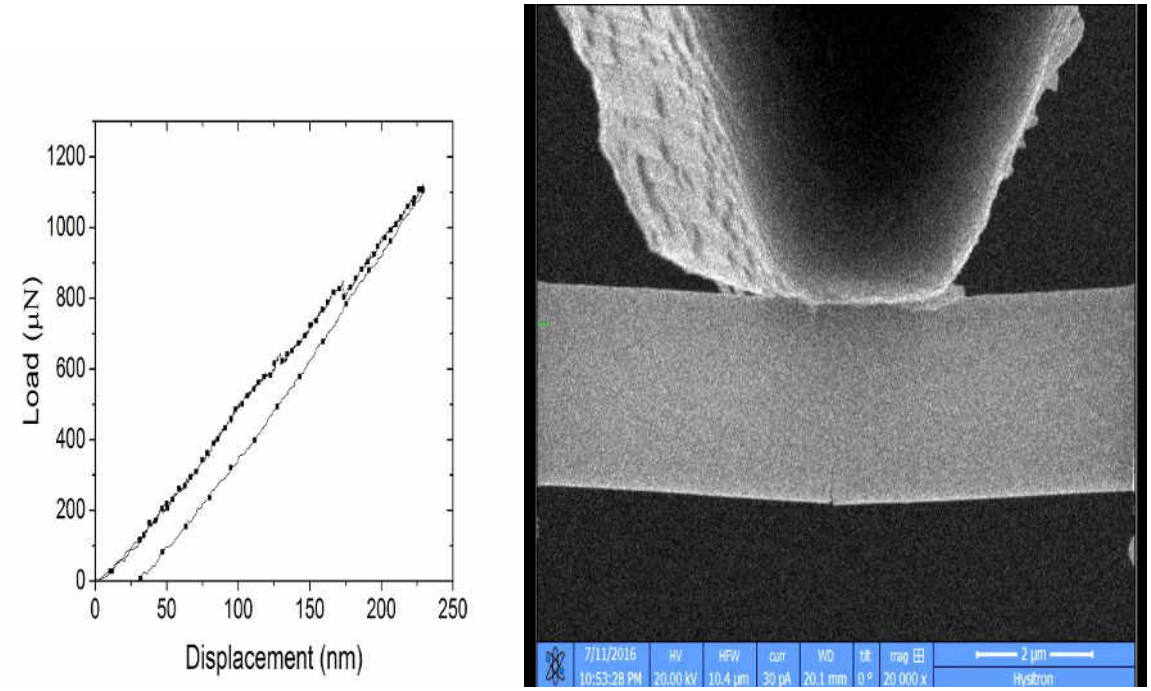


Figure 1 : Three-point bending showing a nanocrack in a 1 μm thick Si beam.[8].

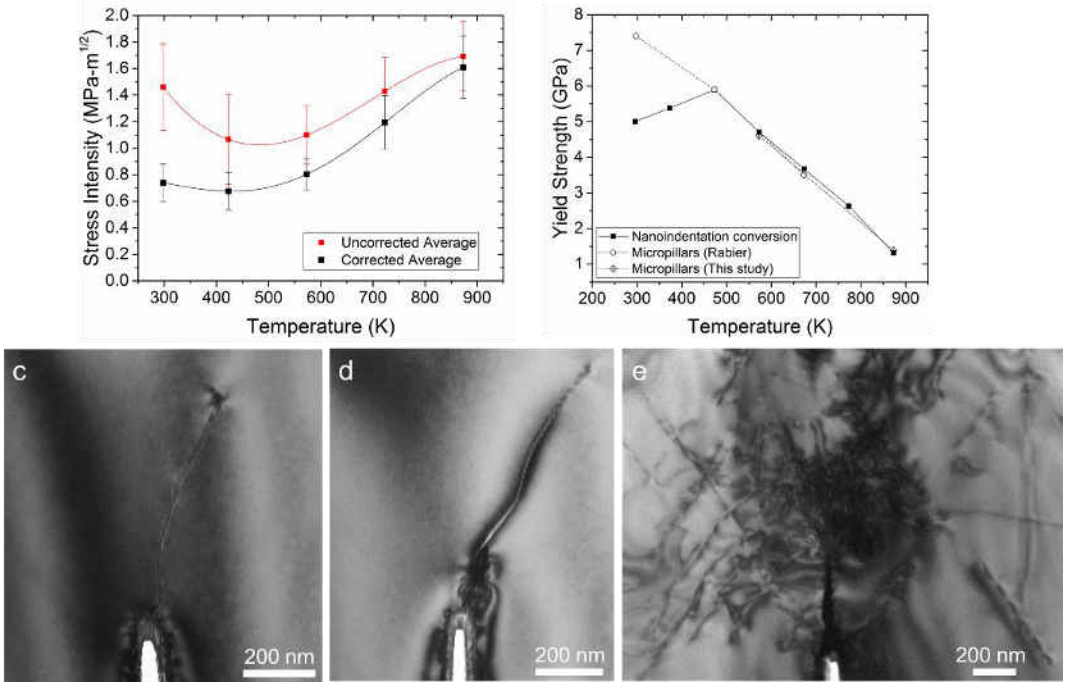


Figure 2: Critical stress intensity at crack arrest for K_{Ic}, σ_{ys} ; Micros for 423,723,873K.

This type of arrested crack can be imaged by transmission electron microscopy (TEM) or it can be reloaded for further crack extension. One can establish at what crack arrest condition one would like to image for dislocation content for a given temperature between 300 and 1000K. Preliminary results are shown at three test temperatures in Figure 2. For the 723 K test in Fig. 2(d), there are six dislocations which have been imaged in this g-

vector TEM condition. Assuming these are the only dislocations emitted at this arrest condition, a realistic estimate of the shielding stress intensity from the back force of the dislocation pile-up can be made. As the crack deviated to a typical {111} plane which is also a slip plane for dislocations, this is a reasonable assumption.

It is significant that the pioneering work of Eshelby and Bilby [5] led to shielding estimates of crack tips by Rice-Thomson [9]. This was later used by Nakao [10] using dislocation shielding to quantify its effect on fracture toughness in silicon. While this was accomplished using a two step process of producing nanocracks by nanoindentation, which were then heated, it is now possible to quantify such effects at temperature by the technique above originally formulated by Jaya [11] and modified by Hintsala[8].using *in situ* evaluations. To illustrate this can be utilized as a predictive tool for minimizing time to improved material performance, examples for both silicon and tungsten are discussed. Regarding silicon, substantial evidence has been reported [7,8]. A forthcoming submission illustrates how a relatively simple algorithm using activation energies, activation volumes, and effective shear stresses noted above can be used. An example of use is in figure 3 where the activation energy of H_0 for dislocation nucleation is found from a fit of $\tau^* V^*$ extrapolated to absolute zero.. The linear fit utilizes partial dislocations to 700K and beyond that a mixture of partials and full dislocations. Further calculation with a simple algorithm having parameters easily measured is given in Figure 4. The one high triangular data point is shown twice with the lower more accurate utilizing the bifurcation analysis of Theocaris [12] which reduced by a factor of 2/3 the high point.

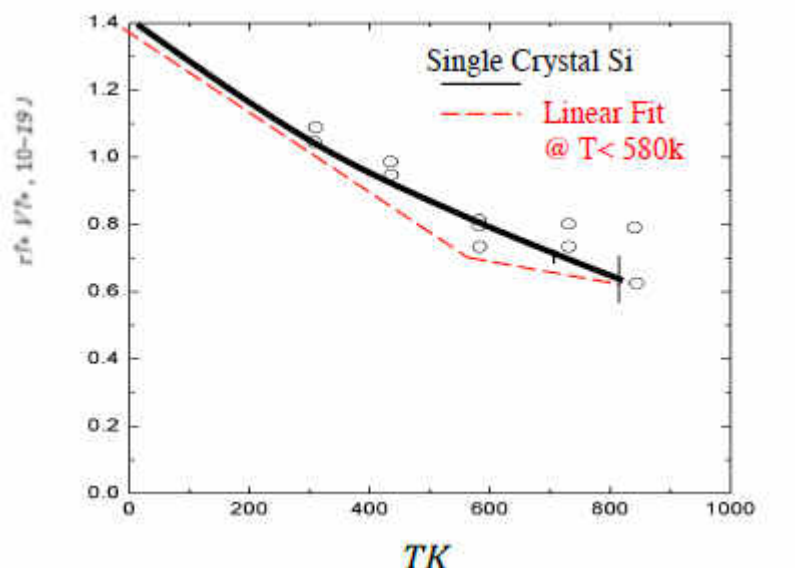


Figure 3: The activation energy, H_0. = 1. 4x 10^{-19} joules.

As a final admission, what is presented here is mostly an experimental technique which could be utilized in conjunction with a larger theoretical simulation program to cross-verify validated experimental and mechanics-based algorithms.

A result is shown for tungsten as given in Figure 4. Here, data on tungsten [13,14],

some of which were pre-strained, are shown. With two thermal activation measurements from two sources [14,15] and two adjustable parameters in the model taken as unity , a reasonaable fit resulted.

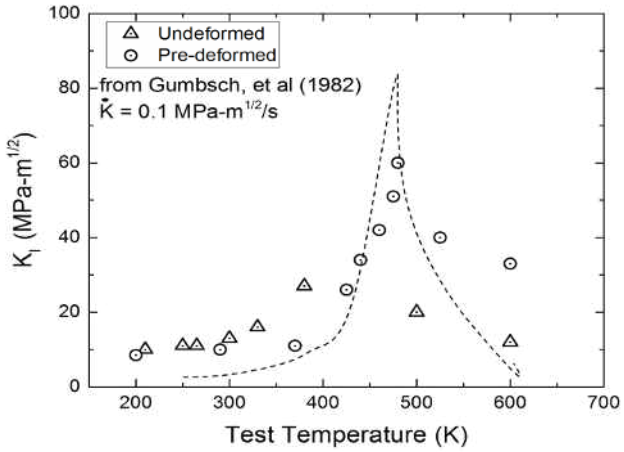


Figure 4: Toughness of W based upon Raffo and Brunner estimates of $\tau^{\bullet}V^{*}$ giving an H_0 of 1.3 x 10^{-19} J.

Conclusions:

- Atomistic simulations give qualitative insight but are currently inadequate for time-temperature.,fracture of complex microstructures.
- In single crystals and single defect states they are increasingly effective.
- Experimentally, nearly all thermally-activated mechanisms can be evaluated at sub-micron scales: τ, τ^*, $v_{dislocation}$, H_0, V^*, K_{IC}, J_I, da/dt.
- The present goal is to facilitate National Lab / University programs for oordinated, reciprocal validation and verification efforts.

References:

1. Hammurabi, Code of Hammurabi.
2. W.A.J. Albert, "Uber Treibseile am Harz" Archive fur Mineralogie Geognosie Berbvau aund Huttenkunde, vol. 10, 1838, pp 215-234.
3. J.H. McCarty and T. Foecke "What Really Sank the Titanic" , Citadel Press, Kensington Publishing Corp. www. Kensingtonbooks.com, March 2008.
4. G.R. Irwin, Plastic Zone Near a Crack and Fracture Toughness, In: *Mechanical and Metallurgical Behavior of Sheet Materials*, 7th Sagamore Ordnance Materials Research Conf. (Syracuse Univ. Res. Inst., N.Y., 1961) pp. 63-68.
5. B.A. Bilby and J.D. Eshelby, Dislocations and the Theory of Fracture, Chapter 2, in *Fracture: An Advanced Treatise*, H.Liebowitz, ed. Vol I. Microscopic and Macroscopic Fundamentals, Academic Press, New York, 1968 pp. 99-182. .
6. P.M. Anderson, J.P. Hirth and J. Lothe, Theory of Dislocations, pp.208-223, Cambridge University Press, New York, N.Y. 10006.
7. E. Hintsala, C. Teresi, and W.W. Gerberich "Linking Nanoscales and Dislocation Shielding to the DBT of Silicon, Metall. & Matl. Trans.A vol47, 2016, pp.5839-5844.
8. E.D. Hintsala, S. Bhowmick, X. Yueyue, R. Ballarini, S.A. Syed Asif and W.W. Gerberich, "Temperature Dependent Fracture Initiation in Microscale Silicon", Scripta Materialia, 130 (2017) pp. 78-82.
9. J.R Rice and R. Thomson, "Ductile Versus Brittle Behaviour of Crystals," Philosophical Magazine 29 (1974) p.73.
10. S.Nakao, T.Ando, M. Shikida, and K. Sato, "Effect of Temperature on Fracture Toughness in a Single-Crystal Silicon Film and Transition in its Fracture Mode". J. of Micromechanics and Microengineeering 18(1) (2008), 015026.
11. B.N. Jaya, V. Jayaram, S.K. Biswas, "A New Method for Fracture Toughness Determination of Al Bond Coats by Microbeam Bending." Phil. Mag. 92 pp.3326-45.
12. P.S. Theocaris, "Complex Stress-Intensity Factors at Bifurcated Cracks," J. Mech. Phys. Solids, 20(1972) 265-279.
13. P. Gumbsch, J. Riedle, A. Hartmaier and H.F. Fischmeister, "Controlling Factors for the Brittle-to-Ductile Transition in Tungsten Single Crystals," Science, 282 (1998) p.1293.
14. A. Hartmaier and P. Gumbsch "On the Activation Energy for the Brittle/Ductile Transition," Physica Status Solidi (b)(1997) 202 R1.
15. P.L. Raffo, "Yielding and Fracture in Tungsten and Tungsten-Rhenium alloys," NASA Technical Note TN D-4567, Lewis Research Center, May 1968.
16. D. Brunner, "Comparison of Flow-Stress Measurements on High-Purity Tungsten Single Crystals With the Kink-Pair Theory", Materials Transactions, JIM, 41 (2000),pp. 152-160.

Overview on Important Research Contributions in Polymer Opto-Electronics

by Show-An Chen, Member EUAS

Short Biography

Show-An Chen was born in Fui-An, China on April 8, 1940 and graduated as B.S. from National Cheng-Kung Univ., Chemical Engineering Department in 1962 and earned his Ph.D. degree in Chemical Engineering from Washington University (St. Louis, USA) in 1969. Since then, he has worked in UniRoyal Inc. (1969-1970) and W. R. Grace Co. (1970-1973) in USA on polymer compatibility and processing, and after returning to Taiwan, has been teaching in National Tsing-Hua University at Chemical Engineering Department as an associate professor (1973-1974), as a professor (1974-date) and as a chairman (1979-1982). He has also been appointed as the honorary chair professor (2010-date) and the director of the Frontier Research Center on Fundamental and Applied Sciences of Matters (2011-2017) of the same University. He is also the editor-in-chief of the Journal of Polymer Research (Springer-Nature) since 1994. He has been conferred the honorary title, Honorary National Chair Professor (2005-date) by the Ministry of Education, Taiwan. He has served as members of academic journal advisory boards, including, Scientific Report (Nature Publishing), Macromolecules, Asia Materials (Nature publishing), Polymer (Elsevier), Polymer Review (Taylor & Francis), J. Macromolecular Science (Taylor & Francis): Physics, Materials Chemistry and Physics (Elsvier).

Research Activities and Publications

His research interests since 1982 to date are in the area of semiconductive polymer and its hybrid with quantum dot for opto-electronics including molecular design, synthesis, structure-property relationship, and device fabrication and physics. He has published 323 research articles in scientific journals with H-index 61 and citation number more than 12,727, and been granted 17 patents (multiple countries). From 1970 to 1983 his research interest was in conventional polymers including structure-property relationship, processing, and polymerization reaction engineering.

Selective Honors and Awards

1982 Academic Research Award, Chung-Shan Academic Foundation
1984 Academic Award in Engineering, Ministry of Educational
1985 Outstanding Research Award, National Science Council (1985-1995)
1995 Distinguished Researcher, National Science Council (1995-2001).
1995 Outstanding Scholarship Award, Foundation for the Advancement of Outstanding Scholarship, (1995-2000)
1999 National Chair in engineering and applied science Award, Ministry of Education (1999-2002)
2000 Member, Asian-Pacific Academy of Advanced Materials
2002 National Chair in engineering and applied science Award, Ministry of Education (2002-2005)
2003 Science and Technology Award, Executive Yuan of Republic of China
2004 TECO technology award, Teco Technology Foundation
2005 life-time National Chair Professor, Ministry of Education, Republic of China (2005 to date)
2006 Outstanding Scholarship Award, Foundation for the Advancement of Outstanding Scholarship (2006-2010)
2007 Outstanding Research Award, Pan Wen-Yuan Foundation
2008 Chairman, Macro Congress 2008, International Union of Pure and Applied Chemistry

(IUPAC), Taipei, Taiwan
2009 Life-time Achievement Award, The Polymer Society, Taipei.
2010 Honorary Chair, National Tsing Hua University (2010.8-2016.7)
2011 Tsing Hua Hou Jin-Duei Senior Chair, National Tsing Hua University (2010.8-2013.7)
2011 Alumni Outstanding Achievement Award, National Chung-Kung University
2013 Fellow, Taiwan Institute of Chemical Engineers (First Time)，
2015 Fellow, The Polymer Society, Taipei, (First Time)
2016 Honorary Doctor Degree (Doctor Honoris Causa), Russian Academy of Sciences (RAS),
2018 Member, EU Academy of Sciences

He is one of the leading experts worldwide in semiconductive polymers, particularly well known for his pioneering concept of "single polymer approach" in molecular design. This seminal method allows high device efficiency (several world records have been set by him) yet simplified device structure and fabrication processes, thus representing a milestone for realizing the large-scale production of the next-generation optoelectronic devices by wet process for applications in lighting, display, light energy conversion into electricity, etc.

The concept of "single polymer approach" was originated from his study in water soluble self-doped polyaniline in 1994, in which protonic acid dopant is grafted onto side chain for preventing dopant diffusion away and phase separation from the conjugated polymer such that molecular level uniformity in conductivity. He then applied this concept to design emitting polymers and charge transporting polymers for polymer organic light emitting diode (P-OLED) by integrating various functional moieties (including electroluminescence, electron/hole transport, interfacial dipole, energy level tuning, and prevention from triplet energy back transfer) into the polymers as side chains for optimizing the performances and simplifying the fabrication process of opto-electronic devices. Extension of this concept to polymer solar cell (PSC) has been made also. This approach has been one of the most prominent methods for molecular design in polymer optoelectronics.

Brief description on his important research findings on semiconductive polymers in fundamentals and applications relating to this approach is given below.

1. Polymer Organic Light Emitting Diode (P-OLED)
(a) The first one introducing electron transport moieties into emitting polymer side chain and obtaining P-OLED with significant efficiency improvement in 2001,[1] which was further evolved into the concept of "single polymer approach" [2-3]. By extending it to high triplet energy polymer [3], he has developed a new polymer with the highest green emission efficiency (in 2006) upon doping with green phosphor. Furthermore, he proposed a gradient HOMO levels in a single blue emitting spiro-polyfluorene chain to provide efficient hole injection leading to the highest blue emitting device in 2008.[4] Further incorporating them into same side chain leads to further promotion to the highest efficiency in 2012 [5].
(b) Pioneering the concept of effective shielding of triplet energy back transfer [6, 7]. The system studied is di-substituted poly(phenylene) doped with green phosphor, in which the triplet energy of the former is lower than the latter and is expected to give no green emission due to back energy transfer. By introducing dense side chains on the polymer as the shield allowing a prevention of triplet energy back transfer and leading to the highest

efficiency in green emission (in 2008 and 2010).
(c) Ingenious design of light emitting polymers able to emit sharp red (R), green (G) and blue (B) lights simultaneously.[8] By employing interaction of stacked hole transport moiety of carbazole with blue emitting polyfluorene segments to yield green emission while maintaining the blue and red emissions from the main chain and grafted red phosphor, respectively, the single polymer able to emit RGB emission simultaneously is obtained, which is suitable for application in full-color display with color filter and has inspired many subsequent researches in white light P-OLED. He has fabricated also a proto-type full color display with this polymer to support its applicability.
(d) Discovering the phenomenon of sequential energy transfer[9]: This phenomenon was found to occur in a thin film of conjugated polymer involving several minor emitting species with various energy levels through various extents of aggregation, leading to the most compact aggregate to receive energy sequentially from the higher energy species. The exploration of the origin of this phenomenon demonstrates why P-OLED gives broad emission spectrum and lower emission efficiency when aggregates form even for an extremely small amount.
(e) Design of electron transport polymer for effective electron injection from high work function metal cathode such as aluminum.[10] By introducing metal ion such as K+ into the cavity of crown-ether grafted onto the side chain of conjugated polymer, the ion then turns into pseudo-metallic state by receiving electron from the crown-ether such that a new electron transport route is created in addition to conjugated main chains, it allows a promoted device ambient stability and high efficiency. The blue emitting polyfluorene device therewith gives the highest external efficiency 5.42% and impressive maximum brightness 54800 nits in 2011, which are far superior to the reported values for the devices with aluminum, cesium, or calcium as the cathode.

2. Polymer Solar Cell (PSC)
(a) The material stated in 1(e) as electron transport layer in PSC possesses multiple functionality (being: optical interference, hole blocking, and interfacial dipole) [11]**.** For the model polymer P3HT blending with fullerene derivative as the active layer, the power conversion efficiency (PCE) is promoted from 5.78% to 7.5%, which was the highest record in 2012 and is still so at the present.
(b)Design the novel low band gap polymer PTB7-Th [12] (which is now the mostly used and commercialized solar cell polymer). When incorporated with the composite cathode fullerene-doped ZnO, the PCE reached 9.35% being the highest record in 2013. In 2014, he used the dual doped ZnO by Indium and fullerene as the cathode [P308], the PCE was further promoted to 10.3%, which for the first time breaks the target 10% set by DOE (USA) and stimulates many researchers launching toward the next target 12%.

3. Water Soluble Self-doped Conducting Polymers.[14,15,16,17] He developed the process of "post-polymerization modification followed by ion-exchange" for preparing the first water-soluble, environmentally stable self-doped polyaniline in 1994 and 1995, which overcomes earlier problems of phase separation and dopant loss via diffusion. Yet, it is unique for its uniform conductivity in molecular level and hence bears significant impacts on the materials developments in the antistatic coatings for submicron e-beam lithography and hole transport layer for P-OLED and PSC. This concept has been granted 3 ROC patents and 4 US patents, and the technology has been applied in developing antistatic materials in e-beam lithography for submicron photomask for integrated circuit by the chemical companies in Japan and developing conductive materials by chemical companies

in Taiwan for conductive layer of touch panel display.

References

1. Y.-Z. Lee, X. Chen, Show-An Chen*, P.-K. Wei, and W.-S. Fann, "Soluble Electroluminescent Poly(phenylene vinylene)s with Balanced Electron and Hole Injections", *J. Amer. Chem. Soc.*, (2001) 123, 2296-2307.
2. M.-C. Hung, J.-L. Liao, Show-An Chen*, S.-H. Chen and A.-C. Su, "Fine Tuning the Purity of Blue Emission from Polydioctylfluorene by End-Capping with Electron-Deficient Moieties", *J. Amer. Chem. Soc.,* (2005), 127, 14576-14577.
3. Y.-C. Chen, G.-S. Huang, C.-C. Hsiao, and Show-An Chen*, "High triplet energy polymer as host for electrophosphorescence with high efficiency", *J. Amer. Chem. Soc*., 128, (2006), 8549-8558.
4. 252. S.-A.Chen*,·H.-H.Lu·and C.-W.Huang, "Polyfluorenes for Device Applications", in Advances in Polymer Science, Vol 212 Polyfluorenes, Volume Editors: Scherf, U. and Neher, D. Springer (2008).
5. C.-W. Huang, C.-L. Tsai, C.-Y. Liu, T.-Hao Jen, N.-J. Yang and Show-An Chen*, "Design of Deep Blue Electroluminescent Spiro-Polyfluorenes with High Efficiency by Facilitating Injections of Charge Carriers Through Incorporation of Multiple Charge Transport Moieties", Macromolecules, *45, 1281−1287 (2012).*
6. S.-P. Huang, T.-H. Jen, Y.-C. Chen, A.-E. Hsiao, S.-H. Yin, H.-Y. Chen, and Show-An Chen*, "Effective Shielding of Triplet Energy Transfer to Conjugated Polymer by its Dense Side Chains from Phosphor Dopant for Highly Efficient Electrophosphorescence", *J. Amer. Chem. Soc.*, (2008), 130, 4699-4707.
7. Y.-K. Huang, T.-H. Jen, Y.-T. Chang, N.-J. Yang, H.-H. Lu, and Show-An Chen*, "Enhancing Shielding of Triplet Energy Transfer to Poly(*p*-phenylene)s from Phosphor Dopant by Addition of Branched Alcohol for Highly Efficient Electrophosphorescence", *ACS Appl. Mater. & Interface*s, 2, 1094–1099 (2010)
8. X. W. Chen, J.-L. Liao, Y.-M. Liang, M. O. Ahmed, H.-E. Tseng, and Show-An Chen*, "High-Efficiency Red-light Emission from Polyfluorenes Grafted with Cyclometalated Iridium Complexes and Charge Transport Moiety", *J. Amer. Chem. Soc.*, (2003), 125, 636-637.
9. K.-Y. Peng, Show-An Chen* and W.-S. Fann, "Efficient Light Harvesting by Sequential Energy Transfer across Aggregates in Polymers of Finite Conjugational Segments with Short Aliphatic Linkages", *J. Amer. Chem. Soc.*, (2001), 123, 11388-11397.
10. H.-H. Lu, Y.-S. Ma, N.-J. Yang, G.-H. Lin, and Show-An Chen*, "Creating a Pseudo-Metallic State of K+ by Intercalating it into 18-Crown-6 Grafted on Polyfluorene as Electron Injection Layer for High Performance of Polymer Light Emitting Diode with Oxygen- and Moisture-Stable Aluminum as Cathode", *J. Amer. Chem. Soc.*, (2011),133, 9634-9637.
11. S.-H. Liao, Y.-L. Li, T.-H. Jen, Y.-S. Cheng, and Show-An Chen*, "Multiple Functionalities of Polyfluorene Grafted with Metal Ion-Intercalated Crown Ether as an Electron Transport Layer for Bulk-Heterojunction Polymer Solar Cells: Optical Interference, Hole Blocking, Interfacial Dipole, and Electron Conduction", *J. Amer. Chem. Soc.*, (2012) 134, 14271−14274.
12. S.-H. Liao, H.-J. Jhuo, Y.-S. Cheng, and *Show-An Chen**, "Fullerene Derivatives-Doped Zinc Oxide Nano-Film as Cathode of Inverted Polymer Solar Cells with Low Band Gap Polymer (PTB7-Th) for High performance", Advanced Materials, *25*, 4766–4771 (2013)
13. S.-H. Liao, H.-J. Jhuo, P.-N. Yeh, Y.-S. Cheng, Y.-L. Li, Y.-H. Lee, S. Sharma, Show-An Chen*, "Single Junction Inverted Polymer Solar Cell Toward Power Conversion Efficiency Up to 10.31% with Bisfullerene Derivative and Indium Dual-Doped Zinc Oxide Nano-Film as Cathode Interlayer", *Scientific Reports,* 2014, 4 : 6813 DOI: 10.1038/srep06813.
14. Show-An Chen* and G.-W. Hwang, "Synthesis of Water Soluble Self-acid-doped Polyaniline", *J. Amer. Chem. Soc.*, (1994), 116, 7939-7940.
15. Show-An Chen* and G.-W. Hwang, "Water-Soluble Self-Acid-Doped Conjugating Polyaniline: Structure and Properties", *J. Amer. Chem. Soc.*, (1995), 117, 10055-10062.
16. S.-A. Chen* and G.-W. Hwang (1996), Structure Characterization of Self-Acid-Doped Sulfonic Acid Ring-Substituted Polyaniline in its Aqueous Solutions and as Solid Film, Macromolecules, (1996) 29, 3950-3955.
17. H.-K. Lin and S.-A. Chen*, Synthesis of New Water-Soluble Self-Doped Polyaniline, Macromolecules, (2000).33, 8117-8118.

Can we create an Intelligent and Evolutionary Robot with a Brain?

by Fuji Ren, Member EUAS

Short Biography

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

For centuries, people all around the world are haunted by one simple question after they realized that human beings are the only intelligent species on this blue planet: ***Can we create an intelligent and evolutionary robot just like us***?

To answer this apparently simple yet actually sophisticated question, we need to go over some fundamental concepts regarding what is an intelligent and evolutionary robot first.

1. A General Blueprint of an intelligent and evolutionary robot

Unlike a conventional robot focusing on the functionality side, an intelligent and evolutionary robot should be centered on a "beautiful mind".

Fig.1 shows such a blueprint of an intelligent and evolutionary robot driven by a "deep brain" which we proposed. In general, its system architecture consists of three layers, i.e., sensing layer, thinking layer and interacting layer. The "deep brain", which grows in the thinking layer, roots deeply on the big data accumulated from the sensing layer, and dominates the interacting layer to perform motions, actions, and even behaviors.

The concepts, content and challenges of each layer are introduced as follows.

(1) Sensing layer

It is responsible for harvesting multi-channel data from the physical world through various heterogeneous types of sensing devices, and then constructs multi-source big database (also known

as corpus) for further processing. Psychologists have already revealed that "multi-channel" and "concurrency" are two important features in human expression. The "multi-channel" mainly refers to text, facial expression, voice, gesture and physiology signals. Information from the same channel could be collected from multi-source devices. For instance, it is quite possible in the real world that information from the gesture channel could be collected through video devices and RF-devices at the same times, making the raw data in an interrupted and chaos way. Therefore, the key challenge of this layer is how to provide structured data and to ensure the quality and quantity of the corpus that could directly affect the success or failure of the information perception.

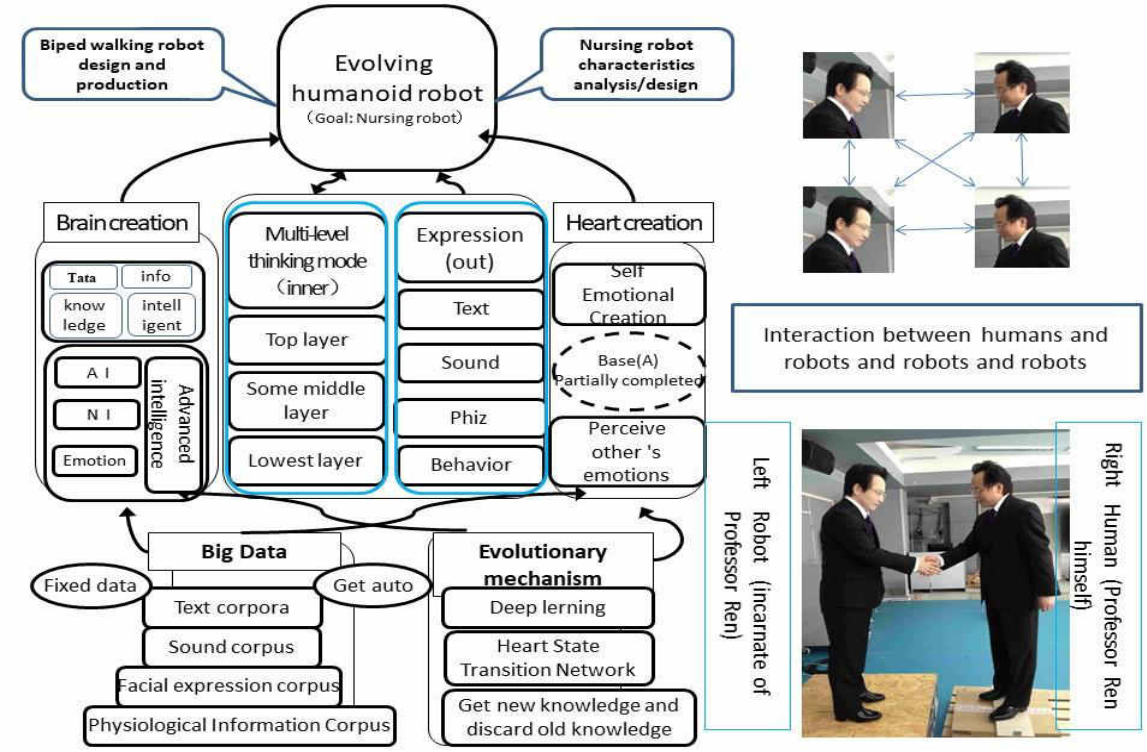


Fig 1. Blueprint of an intelligent and evolutionary robot with a brain

(2) Thinking layer

It is the heart of the robot and in charge of "thinking" through collaborative analysis on the structured multi-modality data. The key challenge is to fuse multi-modal data for extracting the multi-granular collaborative semantic understanding. This challenge can be further divided into the following three levels:

In the representation level, we study the collaborative representation of multi-channel information. And then, the features fused with multi-channel are fed to the semantic understanding layer.

In the semantic understanding level, we study the collaborative context-sensitive semantic understanding models and emotional semantics recognition based on multi-granularity analysis, which uses the large-scale deep neural networks to build the multi-level collaborative and context-sensitive semantic understanding models for multi-modal emotions. And then, the emotional semantics fused with multi-channel is input into the inference layer.

In the inference level, we study the integration of ontology knowledge and implication knowledge, use deep neural network for in-depth computation and symbolic operations and conduct real-time multi-modal and multi-granularity emotional inference, which provides the decision for the natural human-machine interaction.

(3) Interacting layer

It endows the intelligent robot the abilities to interact and evolve. Based on the dynamic interaction model, we study the concurrency and transfer relations between the elements of cognition, intention, decision, expression, etc. We also explore the mapping method from human emotions to machine emotions, and forms the real-time closed-loop feedback mechanism for the emotional generation with multi-channel fusion perception, including vision, auditory and physiological signal, etc.; Lastly, we research on the state concurrency and dynamic feedback mechanism of the natural human-computer interaction loops, develop emotional dynamic generation methods, realize the adaptive intention description and emotional evolution, and provide the models and methods for the natural context perception.

2. Our research progresses on the intelligent and evolutionary robot

In the field of humanoid robot, robot with emotions has been developed rapidly in recent years, REN research lab in Tokushima University have already developed a conversation robot with emotions (Fig. 2). During conversation with human, the robot can detect the emotion of human and make corresponding reply considering both content context and human's emotions.

Fig 2. Conversation robot with emotions from REN lab **Fig 3.** Body structure size collection for robot's

REN research lab has achieved some progresses in emotional assist robot, researchers in the group also study affective computing systems on humanoid robot platform for the mental health problems. The humanoid robot is built according to real person's outlook and body structure. In order to make the perfect approximation, the robot's head adopts reverse would according to real person's size (Fig. 3). The robot's hair is also planted and cut according to real person's style. The researchers think that realistic appearance can improve the acceptance rate.

In order to adopt emotions for the robot, the robot is able to perform several basic emotions, for example six traditional basic emotions including surprise (Fig. 4), sad (Fig. 5) and other three emotions.

Fig 4. The robot simulates surprise

Fig 5. The robot simulates sad

Then we have built a common and personalized fusion mental state transition networks, and developed multi-model emotion conversation model based on that transition networks. In such way, the robot could make some reactions with emotions (Fig.6).

Fig 6. Robot-human emotional conversation

Fig. 7. Female emotional robot

Specifically, REN lab has also built a female emotional robot (Fig.7). The female emotional robot is adopted as a platform to enhance mental health for human. According to user's micro-blog, blog, conversational language, voice, facial expressions and based on emotional interaction the robot could perceive human's mental health status and calculate the heart enrichment degree. The system has the ability to appease, chat with human. The group also developed the emotional robot conversation cloud platform. Key functions of the system include person identification and emotion cognition, gestures and voice interaction, intelligent emotional chat, and other emotional interaction. Emotional robots can be adopted in homes and medical facilities for people of all ages (especially the elderly care), can provide recovery assistant service in specific conditions (autism and depression).

3. Conclusion and Future

In this article, we present some of our recent research results on endowing a robot with intelligence and the ability to evolve. We first describe in detail about a pervasive blueprint of an intelligent and evolutionary robot driven by a "deep brain". Then we briefly introduce our research progresses on the intelligent and evolutionary robot from different aspects.

Contributions to Evolvable Assembly Systems

by Mauro Onori, Member EUAS

Short Biography

Appointments

Head of Department, Production Engineering, Sept. 2013-
Professor, Chair of Adaptable Systems, Oct.2010
Associate Professor , 2008
Assistant Professor , February 2001.
Editorial Board member/Reviewer, Assembly Automation Journal, MCB University Press,UK.

Academic Degrees

02.2001	*Docent (Asst. Professor), KTH, Stockholm, Sweden.*
12.1996	*Teknologie Doktorsexamen (PhD), KTH, Stockholm, Sweden.*
12.1993	*Teknisk Licentiat, KTH, Stockholm, Sweden.*
10.1984	*Master of Science (M.Sc.), Loughborough Univ.of Technology , Leics. UK*
10.1983	*Bachellor of Science (B.Sc.) , 2nd Class Honours, The Univ. of Sussex, England.*

Publications

Publications in peer-reviewed International Conference proceedings and Journals = 150+.
Published peer-reviewed Book chapters, both national & international editorials = 10.
TOTAL no. of Publications = 160+.

Awards

Outstanding Journal article of the year, Emerald Press, UK, 2013
Japan Robot Association Award, JARA-Japan Robot Association, Japan, 1996
Highly Commended Award, Literati Awards for Excellence, MCB Univ. Press, 2001
BASYS 2006, 2nd Best Paper Award, 2003
Karlebo Prize, KTH, Sweden, 1994

Accepted major R&D Proposals (1996-to date)

1996-2000, HFAA, Hyper Flexible Automatic Assembly, PROPER financed Research network; coordinator and main proposer.
1999-2001, SHARC, Standardised Hybrid Assembly with Reactive Capacity, 4th Framework, European Commision Growth project, Steering Committee member and main proposer with IVF
2000-2003, Assembly-Net, European Network for Precision Assembly Technologies, 5th Framework, European Commision Growth project , G1RT-CT-2001-05039, Steering Committee member and main author of proposal.
2003, STINT Scolarship, Development of Evolvable Assembly paradigm with UNINOVA, Portugal, July 2003.
2003-2005, E-Race, E-Space for Collaborative Manufacture od Reconfigurable Assembly Cells, EUREKA EC project , co-member, main proposer TQC, UK
2004-2009, EUPASS, Evolvable Ultra Precision Assembly Systems, 6th Framework European Commision Integrated Project, NMP-2-CT-2004-507978, Project Manager and main author of proposal.
2005-2009, μSapient, Synergetic Process Integration for Micro & nano Manufacture, 6th Framework European Commision Coordination Action, NMT 033227, project member.
2005-2008, A3-Applied Agile Assembly, Marie Curie Transfer of Knowledge project, 6th EC Framework , Steering Committee member and main author of proposal.

2010-2014, IDEAS, Instantly deployable Evolvable Assembly Systems, NMP-2009-SMALL-3, 7th Framework Programme, European Commission Medium Project, , Project Leader and main author of proposal.
2010-2012, ProFLEX, Production Flexibility Cell; QREN Portugues Natinal Project; Scientific Coordinator
2012-2015, PRIME, Plug & pRoduce Intelligent Mechatronic Environment, 7th Framework Programme, European Commission Medium Project, , sub-author of proposal.
2010-2014, ARES, Autonomous Robot Surveillance; QREN Portugues Natinal Project; Scientific Coordinator
2015-2018, openMOS, open Management Operating Systems, Horizon2020 Demonstration project, European Commission Medium Project, , one of main authors of proposal.

Teaching Merits beyond own University

Formal External Lecturer, Universidade Nova de Lisboa (UNL-DEE), assigned by Prof.Steiger, Portugal
Guest Lecturer, École Polytechnique Fédèrale de Lausanne (EPFL), invited by Prof.Jacot , Switzerland, June-July 2004;
Guest Lecturer, Universidade Nova de Lisboa (UNL-DEE), invited by Prof.Steiger, Portugal, June-July 2003.
Guest Lecturer, KTH Visby, Sweden, 2000-2002
Guest Lecturer, Dalarna University, Courses with Dr.Johansson, Sweden, 2004-2007
Scientific Counselor, IntRoSys S.A. 2005-2010.

Personal Research Profile

My research carreer started as far back as 1985, when early assembly automation research was being conducted at the University of Sussex for Thorn/EMI Robotics. After two years developing new tactile sensors for robots, I was employed at KTH to develop radical vision applications for their Mark II Flexible Automatic Assembly Cell, which succeeded in proving that robot-mounted vision could seriously reduce feeder needs. This work then continued within the Mark III system, in which I also became involved with the Programming & Control solutions. This work led to the Hyper Flexible Assembly project (HFAA-PROPER), four major European Commission projects (SHARC, A^3, EUPASS, IDEAS), and have been given the leading role in writing Assembly Roadmaps for the European Commission projects (Assembly-Net, EUPASS,µSapient).

The work around Evolvability started in 2002 , when I launched the idea of *Evolvable Assembly Systems[1]* being the new paradigm to follow1. This was quickly supported by Prof. José Barata (UNL-DEE, Portugal), who brought novel control aspects into the equation. This basically meant that the term "Evolvable Assembly Systems" was presented and detailed by us and eventually developed into the Evolvable Production Systems (EPS) paradigm with tools, methods, etc.. It has, since its launch in 2002, led to the 6^{th} Framework Integrated Project called *EUPASS*, the Marie Curie project called A^3, and was used as the foundation to three new project proposals within the domain of Adaptive Production Systems at EC level, 7^{th} Framework: *IDEAS, PRIME* and *POPJIM*. Currently the EPS paradigm is entering its standardisation phase through the Horizon2020 project *openMOS*.

Evolvable/adaptive Assembly has now been accepeted as a formal paradigm by the IEEE Industrial Electronics Society (IES), and has been invited to present Special Sessions at IEEE/ISAM, IEEE/ISIE, CIRP, IFAC, and other major international conferences as well as Keynote Speeches (IEEE/ISAM, DET/CIRP, etc.). It has, basically, become an established investigative paradigm.

EPS Fundamentals

There is little doubt that nature's primary strategy is "to develop for change and

1 **"Evolvable Assembly Systems – A New Paradigm?";** M.Onori, Proceedings of the 33rd International Symposium on Robotics (ISR2002); Stockholm, Sweden, Oct.2002.

instability". Not only do all living organisms constantly adapt, even our subsystems require this constant updating: keeping balance requires the body to keep hundreds of small motions active! Nevertheless, engineers have proven to be incredibly reluctant to acknowledge such a succesful approach.

Proposers of production system development have predominatly opted for the "predictive" approach: use knowledge of current products, technologies and markets to design a production system [2] for this one given (fixed) scenario. One basically "predicts" the requirements and lifespan of the given product family and where potential variations may come to be added. This is understandable as industry does not like "unknown scenarios" and tends to enforce this approach. Unfortunately the reality is that no scenario is ever 100% predictable, and it will most certainly change as it is created. Therefore this approach is often supported by the "optimisation" clause: predict – develop - discover changes/malfunctions/etc – optimise - new deviation - optimise…etc. This is an endless loop of sub-optimised solutions. In fact, as pinpointed in earlier publications [(3),(4)], flexible systems may be viewed as sub-optimised solutions as they are relatively precise for a range of products but never tailored to any exact product processes.

The predictive approach actually focusses on known and/or past knowledge. However, production systems are extremely complex, markets are volatile, sub-suppliers dependent on variable transport schemes, etc.: this renders any predicted scenario doomed to fail, and all production engineers and system integrators actually know this. As such approaches focus on predicted product scenarios, and cater for known product ranges, they become obsolete within 1-2 product generations. They are seldom re-used, leading to enormous sustainability issues. Flexible systems have attempted to alleviate for such a drawback by creating production system components that have some operational flexibility: they can handle small variations in the given set of equipment operations. Of course there are over 90 definitions of flexibility, denoting how each solution targets a section of the problem area: ability to increase/decrease capability, increase/decrease production volumes, add/remove componets, etc. The truth is that no flexible system has actually succeeded in becoming industrially viable (noteable exception for SMART [5]or JOT[6]).

Since the world is now moving into product personalisation, the product requirements will only become more extreme, more varied and almost ever-changing. The inevitable conclusion is that predictive approaches will never cope with such multiple and continuous variations. They will most definitely not cope with true innovation as this brings entirely new requirements. In order to compensate for such unaccounted deviations, research has developed a large body of work within the field of optimisation ([7],[8]). What happens is that the system development process is overtaken by expensive planners that attempt to counter the limitations. This is, however, like trying to solve a leaking boat with an automatic water pump: manage the immediate danger but the cause is missed. These planning systems have become extremely complex and computationally heavy, without actually solving the main issue of attaining a stable production horizon.

Hence the rise of new, dynamic/evolvable approaches: create systems that are *designed to adapt to changing scenar*ios rather than "fit" into predicted ones: mimic nature. As will be detailed later, several authors have pointed out the pros & cons of such approaches [9], but very few have actually developed such systems. One such paradigm is the Evolvable Production Systems approach [(10),(11)]. The fundamental aspect behind evolvable systems is that it underlines the importance of catering for the *entire chain of stakeholders*, classifying it and linking all levels such that the "evolutionary habitat" is modelled. This has been well described by (Onori et al[11]; Maturana et al[12]) and can be viewed as a further development of Bionic systems (Ueda[13]). This need to model all the stakeholder

requirements and characteristics also underlines the need to have a functional and robust buisness model: most ”selections” taken by the evolutionary processes will be based on such a business model (if we chose to have cost/performance as our main focus).

The bottom line is that production technology solutions that denote flexible characteristics cannot, in any way, be capable of evolutionary characteristics. The EPS paradigm has always underlined the difference and absolute incompatibility between the two approaches. Nevertheless, some literature does adopt the term ”evolvable” when actually meaning ”changing” [14]. This is not quite correct as products do not actually evolve in the true sense of the word because they do not do so *spontaneously* and of their own accord: there is human intervention. Scientifically speaking one should also maintain a certain correctness in relation to the literature and evolvable systems was first defined by other authors in 2002 ([11], [15]).

Evolvable approaches also have to deal with the negative effects of a rather stochastic behavioural evolution: EPS implies that control systems within the production facility actually modify their behaviours *on their own* (but based on well-developed algorithms!). This is one of the reasons why several authors (Ueda[13], Monastori[16], Ribeiro et al[17]), point out that a drawback with evolutionary development systems is emergence: suitable and unsuitable solutions being proposed by the evolutionary process. Hence the need to segregate and eliminate the unsuitable proposals. Once again the difference in underlying philosophy is large: rather than trying to optimise an under-performing solution, evolvable approaches will test and eliminate the least performant solutions (survival of the fittest [18]). In time the very capable solutions will predominate and become de-facto standards for given processes.

The paradigms:

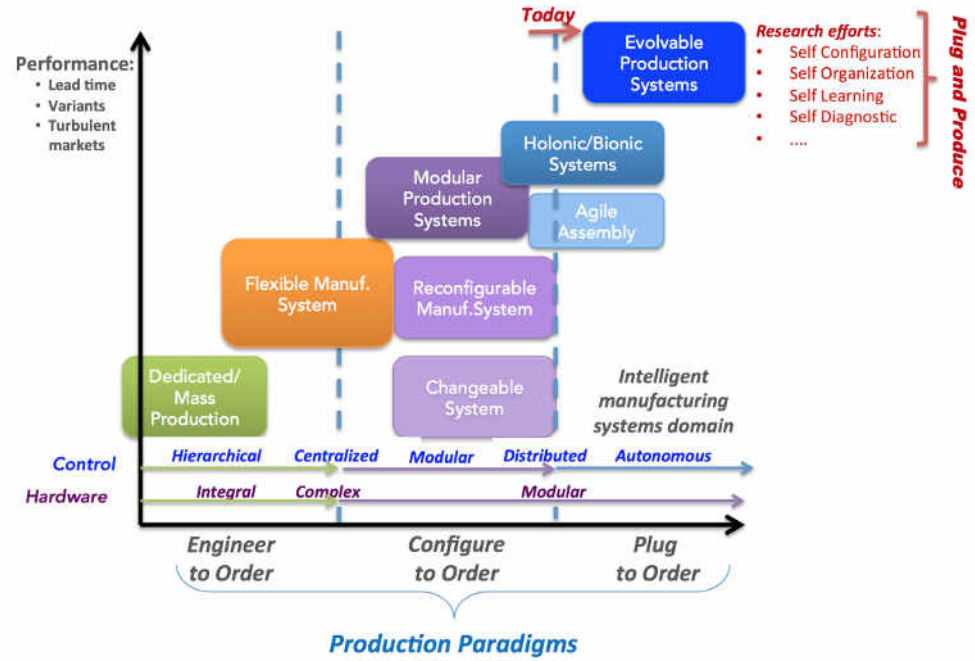


Fig.1.- *Classifying Production Paradigms*

Production paradigms have been developed according to shifts in market behaviours and technological advances. Most remain as loose, rather general terms but a few developed into real paradigms with associated methodologies, architectures and business models. Good examples of such paradigms are mass production, reconfigurable systems

and evolvable production systems. It is almost impossible to list and detail all of the system solutions that have been developed over the years, but a short list of the most well-known ones is as follows:

- Mass Production/Dedicated/Hard automation
- Flexible Automation (Makino[19], Arnström[20])
- Reconfigurable Systems (Mehrabi et al [21], Tolio et al [22], …)
- Changeable Systems (El-Maraghy [23])
- Holonic Systems (Arai [24])
- Agile Automation (Rizzi et al [25])
- Bionic Manufacturing Systems (Ueda [26])…
- Evolvable Production Systems (Ferreira [27], Barata [28], Francalanza et al [29]

It is noteworthy that, at control level, the advent of highly performant, embedded systems have not yet changed the research community's attachment to conventional PLC approaches involving function-block solutions. This may be a determinant factor in the way forward as CPS, Industri 4.0 and Digital Factory all need far more distributed, autonomous solutions that enable self-sustaining approaches: this cannot be achieved by adopting 50 year old computer technology.

This is where architectures become fundamentally important: security, performance at autonomous level and other capabilities cannot be added onto an old architecture and perform suitably. *They have to be designed into the architecture!* An analogy might be as follows: we buy a car from 1960 and add ABS and an airbag system. Does it make it as safe as a car from 2016? No, and any engineer knows why. The same applies to PLCs and factory control: *the new demands need new architectures*.

The second major question is: can we develop solutions on paper and expect them to work in industry? All theoretically defined approaches require real-life demonstrators. This is the only way in which one may collect and analyse the real industrial conditions and requirements. A common criticism of EPS control solutions is that they were not developed step-by-step according to computer science requirements. Even if true, it was a deliberate choice: an approach in which real-life demonstrators became the priority was adopted: by trying the control solutions in real environments, real requirements were collected. This is still ongoing and should be viewed as a bottom-up approach in which industry sets the demands, not science.

Fundamental Foundations

It is interesting to note, as initially listed by [Francalanza 29] that very few paradigms actually develop a "proof-of-concept": a demonstrator production system, and how it came into being. But this is only a part of the problem. New terms remain only terms, a situation which has left many perplexed over time as new "acronyms" turn up without actually having the requirements of being paradigms. Scientifically speaking a paradigm has some fundamental characteristics that need to be met:

- It must lead to re-creatable results; this means that architectures must be developed and detailed, both at hardware and software level. A single system layout represents only a system architecture (one instantiation). What is referred to here are reference architectures.
- It must cover all the sectors that will be influenced: a product approach, a business model for all stakeholders, standardisation approaches, etc. The issue of having an associated business model is probably the most neglected aspect, and the most vital one.
- Must cover all levels of operation: building a system is relatively simple. Ensuring that it is functional and compatible with the control, planning and enterprise-level solutions is fundamental for its industrial acceptance.

***Table 1.0**- Brief summary of paradigms and level of completeness*

Paradigm	Methodology	Reference h/w architecture	Reference s/w architecture	Product/process structures	Business model	Pilot system/ Demonstrator
Mass production	*Yes*	*Yes, basic*	*No*	*No*	*Yes*	*many*
Flexible Manufacturing/ Assembly systems	*Vague*	*Only system architectures*	*Few [23],[24]*	*No*	*No*	*Several ([19],[20])*
Reconfigurable Manuf. Systems	*Vague*	*Not unified*	*Proposed*	*N/A*	*No*	*Yes*
Changeable Systems	*Yes [23]*		*No*	*Yes*	*No*	*N/A*
Holistic Manuf. Systems	*Vague*	*System [24]*	*System[24]*	*N/A*	*No*	*Yes[25]*
Agile Assembly	*No*	*System [26]*	*System*	*No*	*No*	*Yes [29]*
Evolvable Production Systems	*Yes, see [27]*	*Yes, see [28], [37],[38]*	*Yes, see ([30],[31], [38])*	*Yes, ontologies & KB [30]*	*Yes, [32]*	*6, of which 2 industrial [32], [33],[34],[37]*

The need for all of these technological levels to be satisfied was briefly covered in [29], in which a table listing the paradigms and their completeness represents a rare attempt at clarifying the applicability of these approaches. Table 1 is a further development of such a table, in which it becomes clear that very few paradigms are actually applicable, to some degree, in industry.

Finally, and asdetailed by Thomas Kuhn in his famous book [39], the future clearly needs radically new solutions that challenge the limitations of our knowledge. The solutions and tools of yesterday will not solve this and the earlier the entire community agrees to abandon the PLC, flexibility and loosely defined paradigms, the better. *True innovation does not follow known patterns. It breaks into entirely new domains.*

References

1. M.Onori M, J. Barata,Evolvable Production Systems: mechatronic production equipment with process-based distributed control, Proceedings of the IFAC/SYROCO Conference, Gifu, Japan, 2009.
2. H.Akillioglu, P.Neves, M.Onori, "Evolvable Assembly Systems: mechatronic architecture implications and future research", 3rd CIRP Conference on Assembly Technologies and Systems (CATS'10), Trondheim, Norway June 2010.
3. P.Ferreira, N.Lohse, S.Ratchev; "Multi-agent architecture for reconfiguration of precision modular assembly systems", Proceedings of the 5th IFIP WG5.5 International Precision Assembly Seminar; Chamonix, France, SPRINGER 2010.
4. M.Onori, D.Semere, B.Lindberg, (2010), "Evolvable systems : an approach to self-x production", International Journal of Computer Integrated Manufacturing, Taylor & Francis.
5. H. Hitakawa, "Advanced parts orientation system has wide application", Assembly Automation, (1988) Vol. 8 Iss: 3, pp.147 - 150
6. http://www.jotautomation.com/assembly/precision-assembly.html
7. A.Zimmerman, D.Rodriguez, M.Silva; Modelling and optimisation of manufacturing systems: Petri Nets and simulated annealing; Proceedings of the European Control Conference (ECC), Sept.1999, **ISBN:** 978-3-9524173-5-5
8. J.Antony; Simultaneous Optimisation of Multiple Quality Characteristics in Manufacturing Processes using Taguchi's Quality Loss Function; International Journal of Advanced Manufacturing Technology; Jan.2001, Vol.17, Issue 2
9. G Meng, SS Heragu, H Zijm; Reconfigurable layout problem; - International Journal of Production …, 2004 - Taylor & Francis
10. J. Barata, R. Frei, and M. Onori, "Evolvable Production Systems: Context and Implications," in ISIE'07 –IEEE International Symposium on Industrial Electronics, Vigo - Spain.
11. M. Onori, "Evolvable Assembly Systems - A New Paradigm?," ISR2002 - 33rd International Symposium on Robotics, Stockholm, 2002.
12. F.P.Maturana and D.H.Norrie, "A Generic Multi-Agent Mediator for Distributed Manufacturing Systems"; Journal of Intelligent Manufacturing, Vol.7, 1996, 257-270
13. K.Ueda, T.Kito, N.Fujii; Modeling Biological Manufacturing Systems with Bounded-Rational Agents. Annals of the CIRP, 2006; 55/1: 469-472.
14. T.Tolio, M.Sacco, W.Terkay, M.Urgo; Virtual Factory: An Integrated Framework for Manufacturing Systems Design and Analysis; Forty Sixth CIRP Conference on Manufacturing Systems 2013; Elsevier

15. M. Onori och J. Barata, "Evolvable Production Systems: new applications in mechatronic production equipment," i *Industrial Electronics (ISIE),* 2010, s. 2653-2657
16. L.Monostori ; “Towards adaptive and digital manufacturing”; Annual Reviews in Control, 34 (1). pp. 118-128.
17. L. Ribeiro, J. Barata, J. Ferreira; “An Agent-Based interaction-oriented shop floor to support emergent diagnosis”; Proceedings of 8th International Conference on Industrial Informatics (INDIN); Osaka,Japan; July 2010.
18. J. Dias Ferreira, L. Ribeiro, M. Onori, and J. Barata, “Challenges and properties for bio-inspiration in manufacturing,” *IFIP AICT, Technolog- ical Innovation for Collective Awareness Systems, L. Camarinha-Matos*, vol. 423, pp. 139–148, 2014.
19. H.Makino, T.Arai; New Developments in Assembly Systems; Keynote Speech, Annals of the CIRP Vol. 43/2/1994
20. Amstroem, A. and Grondahl, P.,1988, Advantage of SubBatch Principle in Flexible Automatic Assembly as Used in the IVK-KTH Concept Mark 11, CIRP Annals 37/1,9-12.
21. M.G.Mehrabi, U.G.Ulsoy, Y.Koren; Heytler,P.; Trends and Perspectives in flexible and reconfigurable manufacturing systems; Journal of Intelligent manufacturing 13 (2), 135-146
22. T.Tolio, D.Ceglarek, H.A.ElMaraghy, J.Vancza; SPECIES—Co-evolution of products, processes and production systems; CIRP Annals - Manufacturing Technology, Volume 59, Issue 2, 2010, Pages 672–693
23. H.A. ElMaraghy, “Changeable and reconfigurable manufacturing systems”, Springer, London, 2009.
24. T.Arai, Y.Aiyama, M.Sugi, J.Ota; Holonic Assembly System with Plug and Produce, Computers in Industry, 46, 3, 289/299 (2001).
25. A.A.Rizzi, J.Gowdy, R.L.Hollis; “Distributed coordination in modular precision assembly systems”, International Journal of Robotics Research, Vol.20, No.10, pp.819-838, October 2001.
26. P.Ferreira, N.Lohse, S.Ratchev; “Multi-agent architecture for reconfiguration of precision modular assembly systems”, Proceedings of the 5th IFIP WG5.5 International Precision Assembly Seminar; Chamonix, France, SPRINGER 2010.
27. J. Barata, *"Coalition based approach for shopfloor agility - A multiagent approach"*: Edições Orion, 2005.
28. M. Onori, N. Lohse, J. Barata, C. Hanisch: *The IDEAS project: Plug & produce at shop-floor level*. Assembly Automation 04/2012; 32(2).
29. E.Francalanza, J.Borg, C.Costantinescu; Development and evaluation of a knowledge-based decision-making approach for designing changeable manufacturing systems; CIRP Journal of Manufacturing Science and Technology, July 2016
30. J.Ferreira, L.Ribeiro, P.Neves, H.Akillioglu, M.Onori, J.Barata; Visualisation tool to support multi-agent mechatronic based systems; Proceedings of the IECON 2012, 38th annual conference on IEEE Industrial Electronics Society
31. S.Cavin, P. Ferreira, N.Lohse; Dynamic skill allocation methodology for evolvable assembly systems; Proceedings of the 11th Int.Conference on Industrial Informatics, INDIN 2013; ISBN: 978-1-4799-0752-6
32. A. Maffei, “Characterisation of the business models for innovative, non- mature production automation technology,” Ph.D. dissertation, KTH, 2012.
33. M. Onori, J. Barata Oliveira: *Barata, J.: Outlook report on the future of European assembly automation. Assembly Automation 30(1), 7-31*. Assembly Automation 02/2010; 30(1).
34. A. Maffei, M. Onori: *Evolvable Production Systems: Environment for New Business Models*. Key Engineering Materials 02/2011; 467.
35. L. Ribeiro, J. Barata, M. Onori, C. Hanisch, J. Hoos, R. Rosa: *Self-organization in automation - The IDEAS pre-demonstrator*. 11/2011; DOI:10.1109/IECON.2011.6119747
36. J. D. Ferreira, *Bio-inspired Self-Organisation in Evolvable Production Systems*. Tekn. Lic. dissertation, Royal Institute of Technology, Sweden, 2013.
37. J. D. Ferreira, Luis Ribeiro, Hakan Akillioglu, Pedro Neves, Mauro Onori: *BIOSOARM: a bio-inspired self-organising architecture for manufacturing cyber-physical shopfloors*. Journal of Intelligent Manufacturing 09/2016;
38. H.Akillioglu, P.Neves, M.Onori, (2010), “Evolvable Assembly Systems: mechatronic architecture implications and future research”, 3rd CIRP Conference on Assembly Technologies and Systems (CATS’10), Trondheim, Norway.
39. T.S.Kuhn, The Structure of Scientific Revolutions. 3rd ed. Chicago, IL: University of Chicago Press, 1996.

Two Themes in Holomorphic Dynamics

by Mikhail Lyubich, Member EUAS

Short Biography

Education

MS 1980, Kharkov State University. Thesis: "Entropy of rational maps"
PhD 1984, Tashkent State University. Thesis: "Dynamics of rational maps"

Main field of interest

Analytic Low-Dimensional Dynamics, complex and real.

Positions

Institute for Math. Sciences and Math. Dept. at Stony Brook
(Feb 1990 Assistant Professor, Sept 1990 Associate Professor,
Sept 1994 Professor)
Sept 1995 - 2004: Deputy Director of the IMS
2002 - 2007: Professor and Canada Research Chair
at the University of Toronto
Sept 2004 – 2007: Co-Director of the IMS
Sept 2013 – 2016: Chair of Stony Brook Math Dept
Sept 2007 - current: Director of the IMS
2017: SUNY Distinguished Professor

Memberships

Member of the St Petersburg and American Math Societies
Fellow of the American Math Society (Inaugural Class)
Member of the Brazilian and EU Academies of Sciences.

Awards

Prize of Leningrad Math. Society 1987
Alfred P. Sloan Research Fellowship 1991-1994
NSF grants 1991-2019
NSERC grant 2003-2008
Guggenheim Fellowship, 2002 - 2004
Jeffery-Williams prize of the Canadian Math. Society 2010

Selected invited lectures

Plenary address at the ICM-14, Seoul (2014)
Invited address at ICM-94, Zurich (1994)
Plenary address at the V Latin American Congress of Mathematicians, Barranquilla (2016)
Invited address at the International Congress in Mathematical Physics, London (July 2000)
Invited address at the First Latin American Congress of Mathematicians, IMPA (July 2000)
Plenary address at the annual AMS meeting in Washington, DC (Jan 2000)
Plenary address at the joint meeting of FSM and CMS, Toulouse (July 2004)
Plenary address at the annual CMS meeting in Ottawa (Dec 2013)
Jeffery-Williams Prize lecture at the Meeting of the Canadian Math Society, June 2010

Series of Balzan-Palis Symposia at IMPA (Rio de Janeiro) and IHP (Paris), 2012- 2015
Invited speaker at birthday conferences for Bodil Branner (Holbaek 2003), Eric Bedford (Bloomington 2008), Pavel Bleher (Amherst 2017), Leonid Bunimovich (Banff 2009 and Amherst 2017), Robert Devaney (Tossa de Mar 2008), Adrien Douady (Paris 1995 and 2006), John Hubbard (Paris 2005 and Bremen 2015), Yulij Ilyashenko (Moscow 2014), Linda Keen (CUNY 2010), Keith Burns (Provo 2017), Yuri Lyubich (Technion 2006), Nick Makarov (Saas Fee 2016), Welington de Melo (Salvador 2006 and Rio 2016), John Mather (Princeton 2002), John Milnor (Stony Brook 1991 and Cancun 2016), Jacob Palis (IMPA 2000 and Buzios 2011), Dennis Sullivan (New York 2002), Oleg Viro (Stockholm 2008), Alberto Verjovsky (Cuernavaca 2003 and 2013), and Misha Zaigenberg (Grenoble 2016);
at memorial conferences for B.Ya. Levin (Tel-Aviv 2008), Yoccoz (Paris 2017) and A. Douady (Paris 2007);
and at the Lyapunov's 150th anniversary conference (Kharkov 2007).
Magna Conference: A Century of Science: Paving a Better Future, celebrating 100 years of the Brazilian Academy of Sciences, Rio de Janeiro (May 2016)

In recent years I continued to work on various themes of Holomorphic Dynamics in complex dimension one and two. Let me touch upon two of them.

A central theme of the One-Dimensional Holomorphic Dynamics is the Renormalization Theory which is a paradigm for exploring the small scale structure of dynamical and parameter fractal objects. The renormalization transformation is a non-linear operator that relates various scales in a certain class of systems. It is often anticipated that such an operator has a hyperbolic fixed point which captures universal scaling features of the systems in question. Such a result is referred to as a *Renormalization Conjecture*. It is usually difficult to prove (and even to set in a rigorous way), but every advance provides us with a powerful exploration tool. In particular, a celebrated *MLC Conjecture* on the local connectivity of the Mandelbrot set is intimately related to underlying renormalization structures.

The *Mandelbrot set M* is the parameter picture of the complex quadratic family $f_c : z \mapsto z^2 + c$ that can be defined as the set of parameters c for which the critical orbit $(f_c^n(0))_{n=0}^{\infty}$ does not escape to ∞. One of its prominent features is the *main cardioid* comprising those c for which f_c has a neutral fixed point with multiplier $e^{2\pi i\theta}$, $\theta \in \mathbb{R}/\mathbb{Z}$. In this way the cardioid is parametrized by the rotation number θ. The pictures clearly show that M is self-similar near the golden mean rotation number (see Figure 1). Jointly with Dima Dudko and Nikita Selinger, I have developed an underlying *Pacman Renormalization Theory* [DLS] responsible for this self-similarity. We followed up in [DL] to describe a new class of parameters $c \in M$ where MLC holds.

Another theme is dynamics in the complex Hénon family:

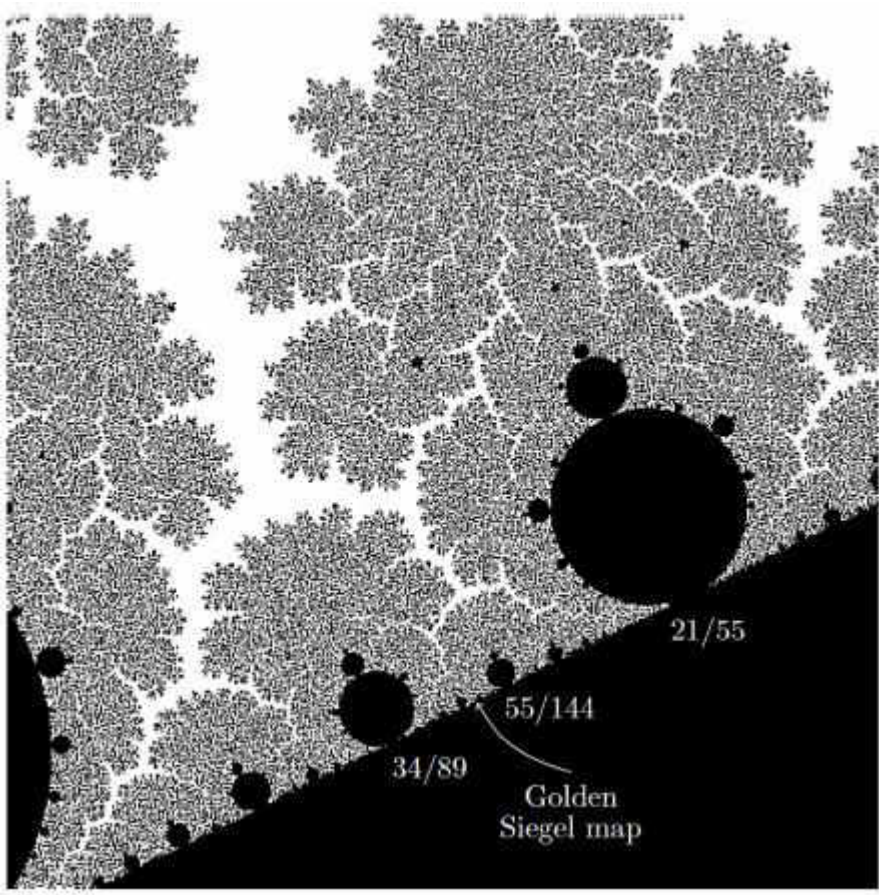
$$F_{c,b} : \mathbb{C}^2 \to \mathbb{C}^2, \ (z.w) \mapsto (z^2 + c - bw, z).$$

Note that $F_{c,b}$ is an *automorphism* of $\mathbb{C}^2$ with complex Jacobian of b. For small b, such a map can be viewed as a perturbation of the one-dimensional quadratic polynomial f_c. The basic theory for the latter is very well developed, and in particular, the dynamics on

the *Fatou set* is completely understood, due to the classical work of Fatou, Julia and Siegel, completed by Sullivan in the early 1980s. Namely, the classics showed that any periodic component of the Fatou set is either an attracting or parabolic basin, or else a rotation domain, while Sullivan's Theorem asserts that any component of the Fatou set is eventually periodic.

An exploration of periodic Fatou components for Hénon maps was originated in the work by Bedford and Smillie in the 1990s. In a recent work with Han Peters [LP1], we have ompleted this study for *substantially dissipative* Hénon maps (when $|b|<1/4$) classifying these components as "attracting", "semi-parabolic" and "rotation" domains exactly as the one-dimensional model suggests.

The problem of wandering domains for Hénon maps is very difficult. In fact, it has been recently shown that complex two-dimensional maps (albeit non-invertible and non-dissipative) may have wandering domains [ABDPR]. However, in [LP2] we ruled them out for substantially dissipative maps that admit a dominated splitting over the Julia set (which, informally speaking, gives us a sense of "vertical" and "horizontal" directions in such a way that the map is more contracting vertically than horizontally). Our result yields a complete dynamical picture for this class of Hénon maps.



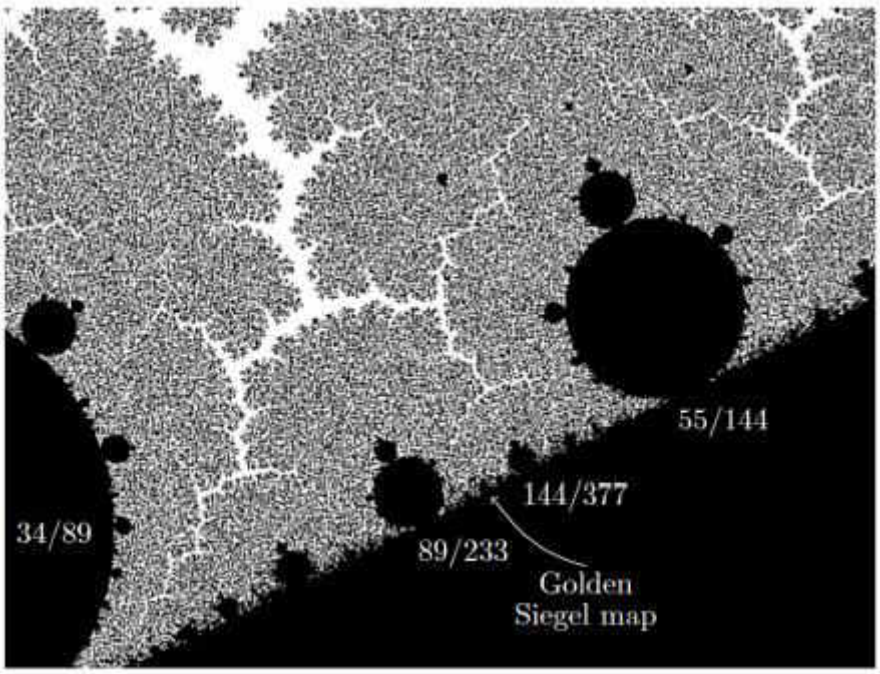


Figure 1. Self-similarity of the Mandelbrot set near the golden mean point.

References

[ABDPR] M. Astorg, X. Buff, R. Dujardin, H. Peters, and J. Raissy. A two-dimensional polynomial mapping with a wandering Fatou component. Ann. of Math., v. 184 (2016), 263 - 313.

[DLS] D. Dudko, M. Lyubich and N. Selinger. Pacman renormalization and self-similarity of the Mandelbrot set near Siegel parameters. Preprint IMS at Stony Brook, # 4 (2017).

[DL] D. Dudko and M. Lyubich. Local connectivity of the Mandelbrot set at some satellite parameters of bounded type. Manuscript in preparation.

[LP1] M. Lyubich and H. Peters. Classification of invariant Fatou components for dissipative Hénon maps. GAFA, v. 204 (2014), 887 - 915.

[LP2] M. Lyubich and H. Peters. Structure of partially hyperbolic Hénon maps. Preprint IMS at Stony Brook, # 2 (2017).

Interaction between the Plasma Atmosphere of the Sun and its Magnetic Field

by Eric Priest, Member EUAS

Short Biography

Current Post: Emeritus Professor of Applied Mathematics, University of St Andrews

Education/Qualifications

Degrees: B.Sc. First Class Honours in Mathematics, Nottingham University (1965)
M.Sc. in Applied Mathematics, Leeds University (1966)
Ph.D. entitled "Magnetohydrodyanmic Neutral point Theory", under T.G. Cowling, FRS, at Leeds University (1969)

Professional History

Career:1968 Lecturer in Applied Mathematics at St Andrews University
1977 Reader in Applied Mathematics at St Andrews
1983 Personal Chair in Theoretical Solar Physics at St Andrews
1992-1997 SERC/PPARC Senior Fellow
1997 James Gregory Professor of Mathematics at St Andrews
2002 Bishop Wardlaw Professor at St Andrews
2010 Retired and made Emeritus Professor
2011 Awarded 2-year Leverhulme Emeritus Fellowship

Prizes, Awards & other Honours:

Named Lectures

1991 Marlar Lecture at Rice University
1998 Lindsay Memorial Lecture at Goddard Space Flight Centre
2000 James Arthur Prize Lecturer at Harvard University
2006 Rosseland Lecture at Oslo University
2006 Robinson Lecture at Armagh
2009 Larmor Lecture at Belfast

Prizes & Awards

1985 Fellow of the Royal Society of Edinburgh
1994 Member of the Norwegian Academy of Sciences
2002 Hale Prize of the American Astronomical Society
2002 Fellow of the Royal Society
2009 Gold medal of the Royal Astronomical Society
2009 Payne-Gaposchkin medal and prize of the Institute of Physics
2013 Honorary DSc at St Andrews University
2016 Birkeland Lecture of Norwegian Academy of Sciences
2017 Hannes Alfvén Medal of European Geophysical Union

Major Committee & Advisory Bodies:

1988-1991President of the International Astronomical Union's Commission on Solar Activity
1990-2008 For three terms - Member of the UK Research Panel on Applied Mathematics
1993-1997 Member of Space Science Advisory Committee of European Space Agency
1996-1998 Convener of the Mathematics Committee of the Royal Society of Edinburgh
1997-2000 Chair of the European Space Agency's Solar Physics Planning Group
1998-2001 Chair of PPARC's Astronomy Committee and co-Chair of its Science Committee
2002-2008 Vice President of the UK Royal Astronomical Society
2007-2010 Chair of Royal Society of Edinburgh's Physics Panel for electing new Fellows
2009-2018 Chair of the Fachbeirat (Science Advisory Panel) of the Max Planck Institute for Solar System Research
2003-present Member of many committees of Royal Society

Publications:

Total number of refereed publications: 465 since 1971.

Total number of citations (from ADS): more than 15200.
4 papers have more than 500 citations and 34 have more than 100 citations (ADS).
Number of research monographs: 3
Number of books edited: 17
h-index = 60
Service to the Community:
He founded an internationally renowned research group on solar theory, currently 30 strong, with many research collaborations across the world.
For many years he led and helped rejuvenate the UK solar physics community (e.g., as chair of the Royal Society's Solar Physics Panel from 1980-1990).
He has mentored and helped many young researchers across the world with their career development
Internationally, he has served on many advisory panels and research committees, such as the international review committee for High Altitude Observatory and the Fachbeirat of the Max Planck Institute for Solar System Research (of which he was a member for 15 years and chair for 7 years). He has also served on many European Space Agency committees and has been on the editorial board of the journal Solar Physics for the past 32 years.

Research

His research involves modelling the subtle interaction between the plasma atmosphere of the Sun and its magnetic field, which is responsible for much of the dynamic behaviour we see both on the Sun and elsewhere in the universe. Research interests include: magnetic reconnection, magnetic instabilities, solar coronal heating, solar flares and coronal mass ejections, the nature and structure of the solar corona, astrophysical MHD.

In 1982 he wrote a research monograph *Solar Magnetohydrodynamics*, which has become a standard in the field and has helped generations of new researchers in Solar Physics. By 2014, the field had become revolutionised by new observations and models, and so the monograph was completely rewritten from scratch as *Magnetohydrodynamics of the Sun.* He also published with Terry Forbes a monograph entitled *Magnetic Reconnection: MHD Theory and Applications.* In 2016, he also edited a book on Science and Religion called *Why Science and Faith Need Each Other.*

(i) **Reconnection.** A major field which he has helped develop is the *theory of magnetic reconnection*, which is a fundamental process in a laboratory, space, solar or astrophysical plasma for converting magnetic energy to other forms (heating, kinetic energy and fast particle energy). This is particularly important in the solar corona where the dominant source of energy is the magnetic field. In two dimensions, an exact solution for magnetic annihilation was discovered (Sonnerup and Priest,1975) and fast Petschek reconnection was put on a firm mathematical foundation (Soward and Priest, 1977). Numerical experiments were carried out on line-tied reconnection (Forbes and Priest, 1982) and flux emergence (Forbes and Priest, 1984), and new families of fast reconnection were discovered (Priest and Forbes, 1986). The triggering of waves by a sudden onset of reconnection was modelled (Longcope and Priest, 2009), and the effect of non-uniform resistivity on fast reconnection was studied numerically (Baty, Priest and Forbes, 2009).

In three dimensions, reconnection is completely different in ways that were modelled in a series of papers. Here reconnection can take place at null points (Pontin et al, 2004; Priest and Pontin, 2009; Pontin et al, 2013) or at separators (Priest and Titov, 1996; Stevenson et al, 2015) (or in the absence of null points at quasi-separators (Priest and Demoulin, 1995; Demoulin et al, 1996). The structure of null points has been categorised (Parnell et al, 1996) and their collapse studied (Parnell et al, 1997).

Different aspects of magnetic topology and its importance in 3D reconnection have been addressed. The possible topologies and their bifurcations from collections of flux sources were categorised (Bungey et al, 1996, 1998), including the topological

behaviour of stable separators (Brown and Priest, 1999) and the differences between potential and force-free models of coronal fields. The distribution of null points above the photosphere was calculated, and topological aspects of global coronal fields was assessed (Maclean et al, 2006, 2007), together with their variation through a solar cycle (Platten et al, 2014).

(ii) Prominences

Malherbe et al (1983) developed current sheet models for prominences. Priest et al (1989) proposed a twisted flux tube model for a solar prominence, while Demoulin et al (1989a, b) and Amari et al (1991) developed it and proposed a 3D force-free model for a prominence. Later, Priest et al (1991) considered the fibril structure of prominences and Priest et al (1996) put forward a model for dextral and sinistral prominences. Mackay et al (1997) model a filament channel, while Mackay et al (1999) modelled filament barbs and van Ballegooijen et al (2000) put forward a mean-field model for the formation of filament channels.

(iii) Solar Flares

Heyvaerts, Priest and Rust (1977) proposed an emerging flux model for a solar flare, in which small flares are produced by emerging flux and the release of stored energy from a much wider region is triggered by emerging flux in large two-ribbon flares (see also Priest and Heyvaerts, 1974; Heyvaerts and Priest, 1976).

Hood and Priest (1979, 1980) proposed MHD instability such as kink instability as the cause of eruptions in eruptive flares, erupting prominences and coronal mass ejections. Later, Priest and Forbes (1990) suggested magnetic nonequilibrium instead as the cause, while Forbes et al (1994) developed the model further.

Forbes and Priest (1983a, b) modelled computationally line-tied reconnection during a solar flare as well as the evaporative upflow in flare loops (see also Forbes et al, 1989). They also developed a numerical model for flux emergence (Forbes and Priest, 1984), while Lin et al (1994) proposed models for ribbon motion.

Cargill and Priest (1982) suggested that the heating in flare loops was created by magnetic shock waves associated with reconnection. A topological analysis of the breakout model was made (Maclean et al, 2004), while Kliem et al (2014) compared catastrophe and instability for flux rope eruption. Zipper reconnection was proposed as a mechanism to build up the twist in an erupting flux rope (Priest et al, 2016; Priest and Longcope, 2017; Threlfall et al, 2019).

(iv) **Coronal Heating**

Heating the corona to a million degrees K compared with the solar surface temperature of 6000K is one of the major unsolved puzzles in astrophysics. Several possible mechanisms have been proposed and developed by Eric Priest and his collaborators. The two main strands of theory are by magnetic waves carrying their energy from below and by many small current sheets forming in the corona and dissipating their energy by reconnection and ohmic dissipation.

Heyvaerts and Priest (1983) suggested phase mixing as a way of dissipating the energy of Alfven waves in a nonuniform medium. Browning and Priest (1984) analysed Kelvin-Helmholtz instability in such waves, while Inverarity and Priest (1995) developed a model for turbulent wave heating.

Heyvaerts and Priest (1984)suggested that dissipation in many small current sheets could be described in terms of turbulence theory; at the same time they proposed that magnetic helicity (which had been proposed by Taylor in connection with laboratory machines) is important in the evolution of the solar corona, so that it is conserved during the reconnective dissipation in many small current sheets, and that if it becomes too large magnetic eruptions will occur, which represent the way that the corona expels magnetic helicity when it builds up too much. Later, Browning and Priest

(1986a, b) applied it to coronal arcades and closely packed tubes, while Dixon et al (1989) and Vekstein et al (1991) generalised Woltjer's minimum energy principle. Heyvaerts and Priest (1992) developed it into a self-consistent model for coronal heating.

Priest et al (1994) suggested that coronal X-ray bright points are heated by reconnection that is driven by the emergence or cancellation of photospheric magnetic fields, and the model was developed by Parnell et al (1994, 1995). Also, Priest et al (1997, 2000) showed how different coronal heating mechanisms produce different temperature profiles in coronal loops.

Priest, Heyvaerts and Title (2002) developed a flux tube tectonics model for coronal heating in many small current sheets as a development of Parker's nanoflare braiding model in which current sheets form at the myriads of separatrix current sheets that separate the flux that originates from many small photosopheric sources. Here simple motions of the sources forms current sheets rather than relying on the complex braiding motions that Parker had envisaged. Later, Priest, Longcope and Heyvaerts (2005) modelled coronal heating at separators and separatrices, while Close et al (2005) estimated coronal flux recycling times.

(v) **Coronal Loops and Current Sheets**

Coronal loops and current sheets are building blocks of the magnetised solar corona, and many aspects of their structure and behaviour have been studied.

The basics for the structure of coronal loops were outlined in Priest (1986). Their thermal equilibrium has been modelled (Hood and Priest, 1980; Wragg and Priest, 1981, 1982; Steele and Priest, 1990, 1991, 1994), together with siphon flows (Cargill and Priest, 1980), thermal instability (Wragg and Priest, 1982) and MHD instabilities (Hood and Priest, 1981; Hood et al, 1982). The structure of untwisted and twisted flux loops has been modelled by Browning and Priest (1982, 1983), as well as their shape (Browning and Priest, 1986), their nonequilibrium (Browning and Priest, 1984), their eruption (Browning and Priest, 1986), and the 3D response to twisting (Reale et al, 2016).

The formation of current sheets has been modelled between approaching dipoles (Priest and Raadu, 1975), during flux emergence (Tur and Priest, 1976), in force-free fields (Vekstein et al, 1991, Bungey and Priest, 1995) and in a sheared field (Vekstein and Priest, 1993). The nature of thermal instability in a current sheet has been considered (Smith and Priest, 1977), as well as their internal structure (Milne and Priest, 1981) and their evolution following the onset of enhanced resistivity (Forbes et al, 1982). Current sheet models for prominences have been proposed (Malherbe et al, 1983a, b; Ridgway et al, 1991,1992). The dynamic collapse of an X-point to form a reconnecting current sheet has been modelled analytically by Titov and Priest (1993).

(vi) **Laboratory Plasmas, Geophysics and Astrophysics**

Applications of MHD lessons from solar physics have been sought in a variety of laboratory, space and astrophysical environments. Forbes et al (1982) modelled reconnection in geomagnetic substorms. Dixon et al (1989) modelled relaxed states in a spheromak.

Heyvaerts and Priest (1989) modelled a non-Keplerian magnetic accretion disc with a magnetically heated corona, while Heyvaerts et al (1996) considered the interaction of a turbulent disc with embedded magnetic fields. Meerson et al (1993) developed a nonlinear theory for radiation-driven thermal instability. Vekstein et al (1994) considered the effect of magnetic dissipation by reconnective relaxation in astrophysical jets. Tsinganos et al (1992) and Lima et al (1996, 2001) proposed new models for stellar MHD winds. Martin et al (1997) modelled Alfven wave support of a dwarf molecular cloud. Wilmot et al (2005) considered low-order stellar dynamo models.

Recent Contributions in Applied Medicine

by John Forrester, Member EUAS

Short Biography

Work Address: *(1) Division of Applied Medicine, University of Aberdeen, Room 4.23, Institute of Medical Sciences, Foresterhill, Aberdeen, AB25 2ZD, Scotland UK*
(2) Lion's Eye Institute, University of Western Australia, Verdun Drive, Nedlands, Perth WA 6018

UNIVERSITY AND MEDICAL EDUCATION

(a) Degrees and other qualifications

1970	*MB, ChB Glasgow University*	
1975	*FRCS(Ed)*	*Royal College of Surgeons, Edinburgh*
1980	*MD(HONS)*	*Glasgow University*
1985	*FRCS(G) Royal College of Physicians and Surgeons, Glasgow*	
1990	*FRCOphth*	*Royal College of Ophthalmologists of the UK*
1998	*FMedSci Academy of Medical Sciences*	
2003	*FRSE*	*Fellow of the Royal Society of Edinburgh*
2009	*FIBiol*	*Fellow of The Society of Biology (formerly The Institute of Biology)*
2009	*FARVO Fellow of ARVO (Association for Research in Vision and Ophthalmology)*	

(b) Academic Distinctions

1976	*Piggott-Werner Memorial (MRC) Travelling Fellowship*
1977	*London Hospital Prize for Original Research in Ophthalmology*
1977	*Middlemore Award (BMA)*
1989	*British Diabetic Association State of the Art Lecture*
1990	*Nettleship Award (for best research in previous 3 years)*
1990	*Visiting Professor, University of Western Australia*
1991	*Duke Elder Medal*
1991	*Ida Mann Medal*
1992	*Award of Excellence, University of Aberdeen*
1993	*Richardson Cross Medal*
1994	*Honeyman Gillespie Lecture*
1997	*Craig Lecture, Queen's University, Belfast*
1997	*British Diabetic Association State of the Art Lecture*
1997	*Spinoza Professor, University of Amsterdam*
1999	*Ernest Finch Professor University of Sheffield*
2000– 2001	*Master, Oxford Ophthalmological Congress*
2004	*Kimura Lectureship, San Francisco*
2005	*The Experimental Uveitis Research Award – German Uveitis Patient Interest Group*
2005	*Ophthalmic Research Lecture EVER*
2006	*Dr William Mackenzie Memorial Commemoration Lecture, Glasgow*
2006	*Distinguished Lecture Series, Cole Eye Institute, Cleveland Meeting, USA*
2007	*The Doyne Memorial Lecture, Oxford Ophthalmological Congress, Oxford*
2008-	*The Experimental Uveitis Research Award by Deutsche Uveitis Arbeitsgemeinschaft*
2009	*Raine Visiting Professorship – University of Western Australia*
2010	*MDA Medal, Cardiff*
2010	*Mooney Medal, Irish College of Ophthalmologists (200th Anniversary)*
2010	*Bristol Eye Hospital 200th Anniversary Lecture*
2010	*Adjunct Professor, University of Western Australia*
2010	*Visiting Professor, University of Pittsburgh*
2011	*Alcon Research Institute Award*
2011	*International Ocular Inflammation Society - David BenEzra Award*
2012	*Donders Lecturer 2012, Netherlands Ophthalmological Society*
2012	*Rich Distinguished Lecture Series, University of Alabama, USA*

2012 *Visiting Professor, University of Kentucky, USA*
2012 *Mildred Weisenfeld Award 2012*
2012 *Bowman Lecture 2012. Royal College of Ophthalmologists Annual Congress*
2012 *Distinguished Scholar Award, Queen's University Belfast*
2013 *Visiting Professor, University of Melbourne*
2013 *Ian Constable Lecture, University of Western Australia*
2013 *Burgess of Guild, City of Aberdeen*
2014 *Honorary Fellowship Royal College of Physicians and Surgeons of Glasgow*
2014 *Honorary Fellowship Royal College of Ophthalmologists of the UK*
2016 *Neil Della Clinician Scientist Lecture, Australia and New Zealand Retina Society*
2016 *Schlaegel-O'Connor Medal, International Uveitis study Group.*

Present Appointment
September 2011 - *Emeritus Professor, School of Medicine, University of Aberdeen*
Jan 2012 – *Professor of Ocular Immunology, Lion's Eye Institute, University of Western Australia*
December 2013 *– Honorary Professor, University of Edinburgh*
Main Areas of Research

- *Ocular Immunology, Uveitis, Autoimmune Disease*
- *Wound Healing and Experimental Corneal Transplantation*
- *Diabetic Retinopathy, Angiogenesis, Endothelial Cell Function*
- *Age-related Macular Degeneration*
- *Clinical Studies in Uveitis, Translational Research in Ophthalmology, Imaging in Ophthalmology,*

Main Areas of Clinical Activity
Until September 2011, provided tertiary clinical service to NHS Grampian, Aberdeen Scotland in field of Ocular Inflammation. Also provided Vitreo-retinal service to same community.
Since April 2012 have commenced providing clinical uveitis service to Lions Eye Institute, Perth, Western Australia.
Publications
1. Papers: Over 350 peer-reviewed publications in both clinical and basic science research. Published work in 2015/16 is detailed below
2. Reviews: Over 80 major reviews and book chapters / editorials.
3. Books: Six books published including The EYE.
Forrester J V, *Dick A D, McMenamin P, Pearlman, E. and Roberts F (2015) 4th Ed The EYE - Basic Sciences in Practice - Textbook published by Elsevier, Ltd. Publishers*

1 Liu, Y. H. et al. Partial retinal photoreceptor loss in a transgenic mouse model associated with reduced levels of interphotoreceptor retinol binding protein (IRBP, RBP3). Exp Eye Res 172, 54-65, doi:10.1016/j.exer.2018.03.020 (2018).

Organ-specific transgenic membrane expression of hen egg lysozyme (HEL) as a "neo-self antigen" has been used in several models to study immunological tolerance. In this study we report the changes which occur in the B10.BR mouse retina when membrane-bound HEL is expressed in photoreceptors under the control of the promoter for interphotoreceptor retinoid binding protein (IRBP, RBP3). On direct clinical examination of the single transgenic (sTg-IRBP:HEL) mouse fundus, a low-level increase in retinal degeneration compared to non-transgenic controls was observed, presenting as drusenoid deposits and occasional small patches of atrophy. On histological examination, there was an overall shortening of outer segments and loss of photoreceptor nuclei in sTg-IRBP:HEL mice, which was more pronounced in the retinal periphery, particularly inferiorly. The fundoscopically observed lesions did not correlate with the photoreceptor shortening/loss but appeared to be located at the level of the retinal pigment epithelium/choriocapillaris layer and were an exaggeration in size and number of similar age-related changes found in wild type (WT) mice. In addition, neither the atrophic lesions nor the photoreceptor shortening were associated with common retinal degeneration genes, nor were they caused by exposure to light damage since mice housed at both high and low ambient light levels had similar degrees of retinal degeneration. Instead, sTg-IRBP:HEL mice expressed reduced levels of soluble retinal IRBP compared to WT mice which were present from postnatal day16 (P16) and preceded development of photoreceptor shortening (onset P21). We propose that insertion of the HEL transgene in the photoreceptor membrane disrupted normal photoreceptor function and led to reduced levels of soluble IRBP and retinal thinning. A similar phenotype has been observed in IRBP deficient mice. Despite the retinal thinning, the amount of HEL expressed in the retina was sufficient to act as an autoantigenic target

when the mice were crossed to the HEL T cell receptor Tg mouse, since double transgenic (dTg-IRBP:HEL) mice spontaneously developed a severe uveoretinitis with onset at weaning. We suggest that, although membrane expression of foreign transgene products is likely to modify the structure and function of tissues and cells, the technology provides useful models to investigate mechanisms of antigen-specific immunological tolerance

2 Cao, L. et al. Endogenous bioelectric currents promote differentiation of the mammalian lens. J Cell Physiol 233, 2202-2212, doi:10.1002/jcp.26074 (2018).

The functional roles of bioelectrical signals (ES) created by the flow of specific ions at the mammalian lens equator are poorly understood. We detected that mature, denucleated lens fibers expressed high levels of the alpha1 and beta1 subunits of Na(+) /K(+) -ATPase (ATP1A1 and ATP1B1 of the sodium pump) and had a hyperpolarized membrane potential difference (Vmem). In contrast, differentiating, nucleated lens fiber cells had little ATP1A1 and ATP1B1 and a depolarized Vmem . Mimicking the natural equatorial ES with an applied electrical field (EF) induced a striking reorientation of lens epithelial cells to lie perpendicular to the direction of the EF. An EF also promoted the expression of beta-crystallin, aquaporin-0 (AQP0) and the Beaded Filament Structural Protein 2 (BFSP2) in lens epithelial cells (LECs), all of which are hallmarks of differentiation. In addition, applied EF activated the AKT and CDC2 and inhibition of AKT reduced the activation of CDC2. Our results indicate that the endogenous bioelectrical signal at the lens equator promotes differentiation of LECs into denucleated lens fiber cells via depolarization of Vmem. Development of methods and devices of EF application or amplification in vivo may supply a novel treatment for lens diseases and even promote regeneration of a complete new lens following cataract surgery.

3 Voigt, V. et al. Ocular antigen does not cause disease unless presented in the context of inflammation. Sci Rep 7, 14226, doi:10.1038/s41598-017-14618-z (2017).

Ocular antigens are sequestered behind the blood-retina barrier and the ocular environment protects ocular tissues from autoimmune attack. The signals required to activate autoreactive T cells and allow them to cause disease in the eye remain in part unclear. In particular, the consequences of peripheral presentation of ocular antigens are not fully understood. We examined peripheral expression and presentation of ocular neo-self-antigen in transgenic mice expressing hen egg lysozyme (HEL) under a retina-specific promoter. High levels of HEL were expressed in the eye compared to low expression throughout the lymphoid system. Adoptively transferred naive HEL-specific CD4(+) T cells proliferated in the eye draining lymph nodes, but did not induce uveitis. By contrast, systemic infection with a murine cytomegalovirus (MCMV) engineered to express HEL induced extensive proliferation of transferred naive CD4(+) T cells, and significant uveoretinitis. In this model, wild-type MCMV, lacking HEL, did not induce overt uveitis, suggesting that disease is mediated by antigen-specific peripherally activated CD4(+) T cells that infiltrate the retina. Our results demonstrate that retinal antigen is presented to T cells in the periphery under physiological conditions. However, when the same antigen is presented during viral infection, antigen-specific T cells access the retina and autoimmune uveitis ensues.

4 Rajendran, V., Netukova, M., Griffith, M., Forrester, J. V. & Kuffova, L. Mesenchymal stem cell therapy for retro-corneal membrane - A clinical challenge in full-thickness transplantation of biosynthetic corneal equivalents. Acta Biomater 64, 346-356, doi:10.1016/j.actbio.2017.10.011 (2017).

Artificial corneas (keratoprostheses) and biosynthetic collagen-based corneal equivalents are surgical implants designed to ease the global burden of corneal blindness. However, keratoprostheses in many cases fail due to development of fibrous retro-corneal membranes (RCM). Fibrous membranes which develop in the anterior chamber after prosthesis implantation do

so on a matrix of fibrin. This study investigated fibrin deposition and RCM formation after full-thickness collagen-based hydrogel implants and compared them with syngeneic and allogeneic corneal grafts in mice. Fibrin cleared from the anterior chamber within 14days in both allo- and syn-grafts but, persisted in hydrogel implants and developed into dense retro-corneal membrane (RCM) which were heavily infiltrated by activated myofibroblasts. In contrast, the number of CD11b(+) macrophages infiltrating the initial deposition of fibrin in the anterior chamber (AC) after hydrogel implantation was markedly reduced compared to syn- and allo-grafts. Inoculation of mesenchymal stem cells prior to collagen gel implant promoted clearance of gel-associated fibrin from the anterior chamber. We propose that a failure of macrophage-mediated clearance of fibrin may be the cause of RCM formation after collagen-based hydrogel implants and that mesenchymal stem cell therapy promotes clearance of fibrin and prevents RCM formation. STATEMENT OF SIGNIFICANCE: The manuscript addresses the potential value of bone marrow-derived mesenchymal stem cell therapy for retro-corneal membrane (RCM) formation in full-thickness transplantation of biosynthetic corneal equivalents. This work reports the pathophysiological changes in the anterior chamber of the mouse eye following full-thickness recombinant human cross-linked collagen-based hydrogel implants in which persistent fibrin promotes the development of dense RCM. Furthermore, pre-treatment with mesenchymal stem cells reduces RCM formation and enhances corneal transparency.

5 Klaska, I. P., Muckersie, E., Martin-Granados, C., Christofi, M. & Forrester, J. V. Lipopolysaccharide-primed heterotolerant dendritic cells suppress experimental autoimmune uveoretinitis by multiple mechanisms. Immunology 150, 364-377, doi:10.1111/imm.12691 (2017).

Exposure of bone-marrow-derived dendritic cells (BMDC) to high-dose ultrapure lipopolysaccharide for 24 hr (LPS-primed BMDC) enhances their potency in preventing inter-photoreceptor retinoid binding protein: complete Freund's adjuvant-induced experimental autoimmune uveoretinitis (EAU). LPS-primed BMDC are refractory to further exposure to LPS (= endotoxin tolerance), evidenced here by decreased phosphorylation of TANK-binding kinase 1, interferon regulatory factor 3 (IRF3), c-Jun N-terminal kinase and p38 mitogen-activated protein kinase as well as impaired nuclear translocation of nuclear factor kappaB (NF-kappaB) and IRF3, resulting in reduced tumour necrosis factor-alpha (TNF-alpha), interleukin-6 (IL-6), IL-12 and interferon-beta secretion. LPS-primed BMDC also show reduced surface expression of Toll-like receptor-4 and up-regulation of CD14, followed by increased apoptosis, mediated via nuclear factor of activated T cells (NFATc)-2 signalling. LPS-primed BMDC are not only homotolerant to LPS but are heterotolerant to alternative pathogen-associated molecular pattern ligands, such as mycobacterial protein extract (Mycobacterium tuberculosis). Specifically, while M. tuberculosis protein extract induces secretion of IL-1beta, TNF-alpha and IL-6 in unprimed BMDC, LPS-primed BMDC fail to secrete these cytokines in response to M. tuberculosis. We propose that LPS priming of BMDC, by exposure to high doses of LPS for 24 hr, stabilizes their tolerogenicity rather than promoting immunogenicity, and does so by multiple mechanisms, namely (i) generation of tolerogenic apoptotic BMDC through CD14:NFATc signalling; (ii) reduction of NF-kappaB and IRF3 signalling and downstream pro-inflammatory cytokine production; and (iii) blockade of inflammasome activation.

6 Heissigerova, J. et al. The Microbiota Determines Susceptibility to Experimental Autoimmune Uveoretinitis. J Immunol Res 2016, 5065703, doi:10.1155/2016/5065703 (2016).

The microbiota is a crucial modulator of the immune system. Here, we evaluated how its absence or reduction modifies the inflammatory response in the murine model of experimental autoimmune uveoretinitis (EAU). We induced EAU in germ-free (GF) or conventionally housed (CV) mice and in CV mice treated with a combination of broad-spectrum antibiotics either from the day of EAU

induction or from one week prior to induction of disease. The severity of the inflammation was assessed by fundus biomicroscopy or by histology, including immunohistology. The immunophenotyping of T cells in local and distant lymph nodes was performed by flow cytometry. We found that GF mice and mice where the microbiota was reduced one week before EAU induction were protected from severe autoimmune inflammation. GF mice had lower numbers of infiltrating macrophages and significantly less T cell infiltration in the retina than CV mice with EAU. GF mice also had reduced numbers of IFN-gamma and IL-17-producing T cells and increased numbers of regulatory T cells in the eye-draining lymph nodes. These data suggest that the presence of microbiota during autoantigen recognition regulates the inflammatory response by influencing the adaptive immune response.

7 Kuffova, L. et al. High-Risk Corneal Graft Rejection in the Setting of Previous Corneal Herpes Simplex Virus (HSV)-1 Infection. Invest Ophthalmol Vis Sci 57, 1578-1587, doi:10.1167/iovs.15-17894 (2016).

PURPOSE: The "high-risk phenotype" of corneal graft recipients is considered to be related to preexisting vascularization such as that associated with herpes simplex virus-1 (HSV-1) keratitis (HSK). The purpose of this study was to investigate the immunologic mechanisms underlying accelerated corneal graft rejection using a mouse model of HSK. METHODS: Herpes simplex virus type 1 keratitis was induced in BALB/c mice. Syngeneic and allogeneic (C57BL/6 mice) corneal grafts were performed in mice with HSK at different times after infection. Some grafts were performed on HSV-infected CD4 T cell-deficient BALB/c mice. Clinical, histologic, immunologic, and virus detection studies were performed on samples of cornea, draining lymph node (LN), and trigeminal ganglion (TG) cells. RESULTS: Corneal grafts in mice with HSK rejected with higher frequency and more rapid tempo compared with grafts in uninfected mice. In corneas with HSK and vascularization at the time of grafting, both syngeneic and allogeneic corneal grafts failed with similar frequency and tempo. However, in the absence of preexisting inflammation and vascularization, syngeneic grafts were accepted when the grafts were performed at a late time point after HSV infection (42 days), whereas allografts were rejected at this time. In contrast, syngeneic grafts in nonvascularized HSV-infected recipients failed if they were performed within 10 days of HSV infection, an effect that was dependent on CD4 T cells, as demonstrated using CD4 deficient mice. Importantly, a variably sustained but strongly positive anti-HSV T-cell response was detected in allografted HSK recipients with a similar but lesser response in syngeneic hosts. CONCLUSIONS: A previous HSV-1 corneal infection predisposes donor grafts to a high risk of failure by both innate and adaptive immune mechanisms in which an anti-HSV CD4 T-cell response plays a prominent role.

Functional Organic - Inorganic Nanohybrid Materials

by Chang-Sik Ha, Member EUAS

Short Biography

Professor, Dept. of Polymer Science and Engineering, Pusan National University [PNU], Busan 46241, Korea

***Education**:*

1978 B.Sc. (Chemical Engineering), PNU
1980 M.Sc., Korea Advanced Institute of Science and Technology [KAIST]
1987 Ph.D., KAIST

Selective Professional Appointments:

1982 - present Professor, Dept. of Polymer Sci. and Eng., PNU
1988- 1989 Visiting Scholar, Dept. of Materials Eng., Univ. of Cincinnati, USA
1997- 1998 Visiting Scholar, Dept. of Chemical Eng., Stanford Univ.. USA
2003 - 2008 Director, National Research Laboratory of Nano-Information Materials
2004 Visiting Scholar, Dept. of Chemistry, SUNY Buffalo, USA
2010 - 2016 Director, Pioneer Research Center for Nanogrid Materials
2010- 2011 Visiting Scholar, Department of Chemistry, UCLA, USA
2012 Vice President, PNU
2013- 2015 Honorary Professor, University of Queensland, Australia
2016 ~ 2025 Appointed as University Distinguished Professor, PNU
2017 Senior Visiting Scholar, Shanghai Industrial Technology Institute, P.R.China

Selective Professional Services:

Editor-in-Chief, Macromolecular Research (2008 – 2011)
Associate Editor, Composite Interfaces, Advanced Porous Materials(2008 ~ present)
Editorial Board Member (~ present): Soft Nanoscience Letter, Journal of Engineering, Open Journal of Polymer Chemistry, Plastic and Polymer Technology, Journal of Sensor Technology, Journal of Encapsulation and Adsorption Science, etc.
President, The Society of Adhesion and Interface, Korea(2013-2014)
Chairman, Polymer Chemistry Division, Korean Chemical Society(2012)
Vice President, The Polymer Society of Korea (2009)
Vice President, The Korean Institute of Rubber Industries (2004-2005)
Vice President, Asia-Oceania Cyclodextrin League(AOCL) (2007-2009)
Chairman of the East-Asia Meeting(2014-2017), IUPAC Subcommittee on Structure and Properties of Commercial Polymers
Reviewer Board Member (RB) for Polymeric Materials, National Research Foundation of Korea(NRF) (2015-2017)
Foreign Society Membership: Society of Polymer Science, Japan (1991-present), American Chemical Society(1991-present)

Selected Honors and Awards:

Best Paper Award, Korean Federation of Science and Technology Societies(2003.4)
Scientists of the Month Award from Ministry of Science and Technology, Korea (2006. 11)
Busan Municipal City Cultural Award (for Natural Sciences)(2006.12)
Samsung Polymer Science Award, Polymer Society of Korea (2011.4)

Best Researcher Award, Pusan National University, Korea(2007, 2009)
Top 100 National Representative Scientific Result Excellency Award, Ministry of Education, Science, and Technology, Korea/Korea Science and Engineering Foundation (KOSEF)(2009. 7)
Top 50 Basic Science Result Excellency Award, Ministry of Education, Science, and Technology, Korea/National Research Foundation of Korea (NRF)(2013. 9)
Top 11 National Representative Scientific Result Excellency Award, Ministry of Science, ICT, and Future Planning, Korea/ National Research Foundation of Korea(NRF) (2014.7)
SPSJ International Award from the Society of Polymer Science, Japan(2017.5.)
Fellow, Korean Academy of Science and Technology(2004.11 ~ present)
Member, National Academy of Engineering of Korea (2004.11 ~ present)
Member, American Association for the Advancement of Science(2017 ~present)

Publications

He published 720 papers in refereed journals, 72 domestic/international patents (13 applied and 59 registered), 22 books and book chapters. Here are his 10 representative publications in the field of materials chemistry including functional polymers, mesoporous organosilica materials, organic-inorganic nanohybrids with various applications such as organic light-emitting devices, flexible substrates, drug delivery, and metal adsorption, etc.

Organic/inorganic hybrid composites constitute emerging advanced materials since they combine unique properties from the inorganic and organic components. In particular, polymer based hybrid nanocomposites represent a radical alternative to the conventional polymer composites by reinforcing polymers with a second inorganic phase.

Depending on how many dimensions of the dispersed phase are in the nanometer range, one can distinguish three different hybrid nanocomposites. First type of nanocomposite corresponds to the case where the reinforcing phase, in the shape of platelets, has only one dimension on a nanolevel. Polymer-layered silicate (PLS) nanocomposites belong to this class. Second, nanocomposites can also be reinforced by a phase which has only two dimensions in the nanometer scale. This is the case for polymer matrices reinforced by cellulose whiskers and nanotubes, etc. Polymer hybrid nanocomposites can be reinforced by isodimensional phases, which have three dimensions in the nanometer range, such as precipitated silica, silica (or titania) oxides synthesized by the sol–gel process, and silica beads, but also colloidal dispersion of rigid polymers, and many others.

Nanodimension means that the size is pretty close to molecular size. This fundamental length scale dominates morphology and macroscale properties of nanomaterials. This is the reason why nanocomposites are different and worthy of rapidly increasing scientific and technological excitement. The term “nanocomposite” describes a two-phase material; here one of the phases has at least one dimension in the nanometer (10^{-9} m) range. The nanoparticles have at least one characteristic length scale that is of the order of nanometers and can range from essentially isotropic to highly anisotropic needlelike to sheetlike elements. Uniform dispersion of these isotropic and anisotropic nanoscopically sized particles (or nanoelements) can lead to an ultralarge interfacial area between nanoelements, which begins to approach molecular dimensions at extremely low loadings of nanoparticles. Thus, for a system comprised of 1-nm-thick plates, for instance, the distance between plates (considered as discs with a diameter 1 μm) approaches 10 nm at only a few vol. % of plates. This large internal interfacial area and the nanoscopic dimensions between constituents differentiate polymer nanocomposites from traditional composites and filled plastics. The dominance of interfacial regions resulting from the nanoscopic phase dimensions implies that the behavior of polymer-based hybrid nanocomposites cannot be understood by simple scaling arguments that begin with the behavior of traditional polymer composites. Three major characteristics form the basis of the performance of polymer-based hybrid nanocomposites: nanoscopically confined matrix,

nanoscale inorganic constituents, and nanobuilding blocks formed from these constituents.

Here, I would like to describe chronological overview on the topics of polymer hybrid nanocomposites and/or functional organic-inorganic nanohybrid materials that have been done for recent two decades in my laboratory[1].

1. Polymer/layered silicate hybrid nanocomposites

Researchers from Toyota discovered the possibility to build a nanostructure from a polymer and an organophilic layered silicate. After the Toyota's pioneering work, numerous works have been reported to develop new types of polymer-layered silicate (PLS) hybrid nanocomposites. We also developed PLS hybrid nanocomposites based on malleable polyurethane, thermoplastic vulcanizate, polybutylene terephthalate(PBT) and/or its blend with ethylene-vinylene copolymer(EVA), etc. Among many publications reported in our laboratory, the work on the PBT is noteworthy in the sense of enhancing the interfacial adhesion in polymer-based hybrid nanocomposites. When preparing PBT PLS hybrid nanocomposites, we found that epoxy resin as a third component played important roles to improve dispersion of organoclays in the PBT matrix due to the compatibility and interaction between organoclays and the PBT chain.

One of the key findings in my laboratory was to develop biodegradable PLS hybrid nanocomposites. In particular, the aliphatic polyester(APES) based PLS hybrid nanocomposites were recognized to be one of the breakthrough works in the field. The work was the first publication on the biodegradable PLS hybrid nanocomposites in the world. In the work, we measured biodegradability of the PLS hybrid nanocomposites. Before the publication, other researchers always said, "In most cases, properties of PLS hybrid nanocomposites are improved than those of parent polymers that do not have inorganic materials. The improved properties include thermal, mechanical properties, and flame-retardancy, and so on. Biodegradability may be also improved for PLS hybrid nanocomposites." However, our findings showed that the biodegradability of the APES based PLS hybrid nanocomposites was not increased but decreased with increasing contents of organoclays. After publishing the APES PLS hybrid nanocomposites, we further developed thermoplastic starch (TPS) based PLS hybrid nanocomposites and measured their tensile properties and water vapor barrier properties. A series of the works on the TPS PLS hybrid nanocomposites also got a great attention from researchers in the sense that the works dealt with water vapor barrier properties of PLS hybrid nanocomposites for the first time as well as in that they were another brand-new biodegradable PLS hybrid nanocomposite. Chitosan was also a main matrix polymer in my laboratory to develop biopolymer-based nanocomposites.

2. Polymer/graphene oxide hybrid nanocomposites

A few key synthetic polymers that are my favorite polymers for long times include polyimide(PI). In particular, we developed many brand-new transparent and colorless PIs that could be applied for a substrate in flat panel displays such as organic light-emitting devices (OLEDs). PIs are an important class of well-known high-performance step-growth polymers because of their unique physicochemical properties, such as thermal and mechanical stability, controlled dielectric behavior, good adhesion properties, and chemical resistance. Because of these traits, PIs have been used widely in a range of applications, e.g., in microelectronics, aerospace, and membrane science. More recently,

these materials have been used as polymeric components of organic–inorganic hybrid nanocomposite systems that are an important class of new-generation materials that combine the desirable combined properties of inorganic phases, and PI.

Among many works on PI containing hybrid nanocomposites, we conducted a series of noteworthy works on PI/graphene oxide(GO) hybrid nanocomposites mainly with focusing on the improvement of interfacial interaction and enhancing properties.

3. Silica containing polymer nanocomposites and/or functional organic-inorganic nanohybrids

As mentioned in the Introduction, the creation of inorganic–organic hybrid nanocomposites is growing into an important research area because of these materials' distinguished properties, which usually arise from a synergistic effect of the properties of their organic and inorganic components in the resulting hybrid nanocomposites. The advanced properties are usually obtained by distributing nanometer-scale inorganic particles evenly within a polymer matrix. Among the several routes to synthesize these hybrid nanocomposites, perhaps the most prominent one is the incorporation of inorganic nanoparticles into organic polymers using sol–gel reactions. This method allows direct mixing between the inorganic and organic polymers. These hybrid nanocomposites have attracted much interest in the field of materials science because of the ability to control their morphologies and for their enhanced properties — such as mechanical, thermal, and electrical stability and chemical resistance — relative to their organic polymer counterparts by tailoring organic–inorganic segments into the final hybrid nanocomposites. Thus, we intensively investigated on the microstructure and property relationship of PI/silica hybrid nanocomposites via the sol-gel process.

The use of silsesquioxane (SSQ) in the PI/silica hybrid nanocomposites were interesting in the sense of improving the interaction between PI and silica as well as enhancing the properties of the resultant hybrid nanocomposites. The term "silsesquioxane" refers to a wide range of structures that have the general empirical formula $RSiO_{1.5}$, where R is a hydrogen atom or an organic derivative, such as any alkyl, alkylene, aryl, or arylene group or an organofunctional derivative thereof. Unlike silica, silicones, or inorganic fillers, SSQ containing molecules have an organic group in the framework that could make the nanostructure of SSQ containing molecules be compatible with polymers, biological systems, or surfaces. Thus we also intensively studied on the fabrication and application of functionalized SSQ based nanostructured materials including hollow functionalized SSQ nano-materials. In addition, functionalized mesoporous organosilica materials have been also another important subject in my laboratory. In particular, we extensively investigated on organic-inorganic hybrid mesoporous silica materials, or sometimes called as periodically mesoporous organosilicas(PMOs) and their advanced application such as for drug delivery and metal adsorption.

4. Advanced application of polymer-based hybrid nanocomposites and/or functional organic-inorganic nanohybrids.

Though many advanced applications may be expected, we mainly developed polymer based hybrid nanocomposites for low-k materials, organic light-emitting devices (OLEDs), drug delivery systems, and hydrogels. Among such advanced application studies, our noteworthy contributions are on the application of CS-silica hybrid nanocomposites and

PMOs for controlled drug delivery.

In addition, polymethylhydrosiloxane (PMHS) is a siloxane-based transparent liquid with potential use in a wide range of applications owing to its high thermal stability, inertness to air and moisture, solubility in common organic solvents, hydrophobicity, and low surface energy. We also developed various PMHS containing hybrid nanocomposites with natural leaves and/or silica, etc. The PMHS based hybrid nanocomposites showed excellent superhydrophobicity and other interesting properties including oil absorption, metal adsorption, and self-cleaning, etc.

5. Summary of my contribution to the research field of material chemistry and polymer sciences

Organic-inorganic hybrid nanocomposites can cover a broad range of materials consisting of organic materials such as polymers as a matrix and inorganic materials as a dispersant. Organic/inorganic hybrid nanocomposites constitute emerging advanced materials since they combine unique properties from the inorganic and organic components. Inorganic phases are usually dispersed in organic matrix in the nanometer dimension for organic-inorganic hybrid nanocomposites. Furthermore, since the inherent nature of organic materials and inorganic nanomaterials are fundamentally different each other, there are plenty of rooms to investigate the interfacial interaction of organic and inorganic materials in the molecular/nanometer scale, micro/nano-structure and properties of the resultant hybrid materials. Thus a variety of brand-new organic-inorganic hybrid nanocomposites may be expected depending on their future applications, while interesting science may lie under such hybrid nanocomposites, which comes from interface between organic and inorganic materials.

I believe that polymer hybrid nanocomposites and/or organic-inorganic hybrid nanocomposites are among hot topics in material chemistry as well as in polymer sciences and applications. In this sense, my contribution in the research field of the polymer-based hybrid nanocomposites and/or organic-inorganic hybrid nanocomposites may cover the findings of advanced applications of those hybrid or nanocomposite materials for information technology, biotechnology, and environment science, etc. as well as their fundamental physics and chemistry such as the relationship between their micro/nanostructure and properties.

Reference

1. Part of this brief overview was extracted and edited from my article; C.S. Ha, “Polymer Based Hybrid Nanocomposites; A Progress toward Enhancing Interfacial Interaction and Tailoring Advanced Applications,” Chem. Rec. https://doi.org/10.1002/tcr.201700030.

Motivation, Scope and Structure of the 2nd Edition of the Encyclopedia of Computational Mechanics with special Focus on the first two Volumes: Fundamentals

by Erwin Stein, Member EUAS

Short Biography

Univ.-Prof. em. Dr.-Ing. habil. Dr.-Ing. E.h. Dr. h.c. mult.
Institute of Mechanics and Computational Mechanics
Leibniz Universität Hannover, Germany
Studies of Civil Engineering and Mathematics at Polytechnical University of Darmstadt, Germany, Construction and Analysis of wide-spanned Bridges in industry, Promotion and venia legend at the University of Stuttgart, Ordinarius of the Chair of Mechanics and Computational Mechanics of the University of Hannover, Official Inspection Engineer for Structual Engineering in the Land of Lower Saxony
Founder and Curator of the Leibniz exhibitions of the Leibniz Universität Hannover
Honorable Doctor of the Universities of St. Petersburg, Stuttgart, Xuzhou/Beijing and Poznan
Gauß-Newton Congress Medal of IACM, Zienkiewicz Medal of the Polish Ass. For Computational Mechanics (PACM), Ritz-Galerkin Medal of ECOMAS, Awarding with the Verdienstkreuz 1. Klasse des Niedersächsischen Verdienstordens
Honorable-Member of IACM and GAMM
Member of several Academies of Sciences in Germany and Europe
Editorial board-member of 8 international scientific journals
Lead editor of the Encyclopedia of Computational Mechanics (ECM), forthcoming 2ndelectronic edition
425 scientific publications (including 16 books as author, co-author, editor, and/or co-editor) on kinematic, material, and mathematical modeling of technical objects together with computational mechanics, i.e. computer-oriented numerical methods (esp. finite element methods), error analysis and adaptivity, algorithms, and software engineering in continuum and structural mechanics, and application to complex engineering problems. Principal editor of the "Encyclopedia of Computational Mechanics" with 3 volumes consisting of 75 articles on approx. 3.000 pages, published by John Wiley & Sons, Chichester, UK, and also available on the Internet since October 2004. First electronic revision in 2007. Forthcoming second electronic edition in 2016.
Co-editor and member of the Editing Boards of 8 national and international scientific journals 51 DFG research projects, including "Special Research Areas", chairman of "Priority Projects" within Germany, chairman of "Priority Projects" at the University of Hannover and individual research projects.
4 joined research projects, supported by the Volkswagen Foundation, Hannover

Several industrial research projects, mostly concerning the evaluation of damage and failure
Initiation and supervision of 54 doctor theses of students at our Institute and reviews of 30 further doctor theses
Initiation and reviews of 9 habilitation theses of institute members and 4 further habilitation theses at other universities
As a result of nearly 30 years of establishing a school of Computational Mechanics as a new important subject at the Leibniz Universität Hannover, 10 former members of the institute became full professors (with chairs) at German universities, and 13 former members became professors at universities of applied sciences (Fachhochschulen)

The 1st edition of the *Encyclopedia of Computational Mechanics* (ECM1) from 2004 had 3 volumes with in total 68 chapters across 2,500 pages – the 1st volume with 26 chapters on 798 pages for *Fundamentals,* the 2nd with 24 chapters on 830 pages for *Solids and Structures* and the 3rd with 18 chapters on 672 pages for *Fluids* – published by Wiley Inc. with the commissioning editors Erwin Stein for *Fundamentals*, René de Borst for *Solids and Structures*, and Thomas J.R. Hughes for *Fluids*.

The 2nd extensively extended and revised edition (ECM2) in printed and electronic form from November and December 2017 has the same structure as the 1st edition with the three main topics but with two volumes for each of them. *Fundamentals* has 28 chapters, among them 6 new ones with in total 1,188 pages. *Solids and Structures* now has 23 chapters with 1,462 pages, and *Fluids* now has 25 chapters with 1,292 pages, in total 76 chapters across 3,942 pages.

Concepts and novelties of *Fundamentals* are summarized in this report. It may be remarked that the extensive editing tasks with selecting, reviewing, and extensive correspondence with the authors together with the own contributions required high efforts, especially in the years 2016 and 2017.

Vol. 1 & 2 of ECM2 contain related continuous and numerical analysis of the major mathematical models of solid and fluid mechanics, solution methods of algebraic equation systems and computer science. The chapters are structured as discretization methods with finite differences and mostly various discrete variational forms for initial-boundary value problems of partial differential equations, boundary integral equations and further problem-oriented techniques, with mesh-based and meshfree discretizations and the generation and visualization of geometry by various classical and advanced techniques. Also time-dependent parabolic problems and FEMs for the Maxwell equation are included as well as new chapters on uncertainty quantification and related stochastic modeling and solutions.

The joint preface of the editors states: Computer simulation has become the third pillar of science alongside experiments and theory. Computational Mechanics has emerged as one of its greatest successes, having reached a high degree of maturity, reliability and efficiency. It has revolutionized engineering design and analysis, and it is fair to say that every automobile, airplane, ship and train that is manufactured, and almost every consumer product and industrial process, relies heavily on Computational Mechanics methods.

It could and still can be detected quite often, that direct variational approximation methods for analyzing complicated mechanical behaviors of engineering solids, structures and fluids – in the style of classical engineering mechanics – may have considerable shortcomings concerning the existence and the properties of related analytical solutions, e.g. with respect to numerical stability, ultimate loads, as well as material damage in the form of microcracks and microvoids. This also concerns the derivation of proper a priori and a posteriori bounded error estimators as the basis for consistent and optimally adapted mesh-based and meshfree finite element discretizations. The necessary goals are stable and

optimally convergent numerical approximation processes, realized by *Verification*, i.e. using error-based local and global adaptive discretizations. This requires consistent physical and mathematical computational frames. Therefore, *Verification* is a main issue of *Fundamentals*. Whereas the more general and main goal has to be *Validation,* i.e. adaptivity of the mathematical model, especially concerning constitutive equations with material parameters from physical experiments with measurements which have to be identified as well as different types of non-linearities. *Validation* is a main issue in the topics *Solids and Structures* and *Fluids*. Of course, each validation step by model expansion or model reduction has to be accompanied by related verifications in order to achieve sufficiently exact and reliable numerical solutions.

The 11 main topics of *Fundamentals* are: I. Introduction and Survey; II. Finite Difference Methods; III. Classical and Mixed Finite Element Methods; IV. Application to Solids and Structures with Related Materials at Small and Large Deformations; V. Predictive Computational Science as well as Uncertainty Quantifications; VI. Isogeometrical Analysis; VII. Meshfree Approximation Methods; VIII. Wavlet Techniques; IX. Discontinuous Petrov-Galerkin Methods with Applications to Maximal and Parabolic PDEs; X. Boundary-Integral Equation Methods; XI. Algebraic Equation Solvers, Multigrid Methods, Panel Clustering, Domain Decomposition Methods.

In the sequel, the six new chapters in *Fundamentals* of ECM2 are briefly discussed. Two of these treat the mathematics and geometric representations in *isogeometric variational discretizations*; *isogeometric* means the representation of undeformed and deformed geometries with the same shape functions as various types of splines by which high degrees of geometrical continuity, e.g. of thin shells with high continuity properties, can also be achieved for the deformed, e.g. buckled configurations. The mathematical part is authored by T.J.R. Hughes and G. Sangalli and the geometric part by M. Haberleitner, B. Jüttler, M.A. Scott and D.C. Thomas.

Meshfree methods based on level-sets already have a long tradition since the 1980s, but next to more basic benefits, there are some practical and theoretical shortcomings, so far especially for engineering applications. The revised chapter *Meshfree Methods* by A. Huerta, T. Belytschko, S. Fernández-Méndez, T. Rabczuk, X. Zhuang and M. Arroyo contains new variants and algorithms for the representation of discontinuities, e.g. finite cracking particles and fracture, modeled with phase-field methods as well as the propagation of material defects at macroscales and developing damage and local failure at microscales. A powerful variant of meshfree test- and trial-functions is presented in the new chapter: the *Reproducing Kernel Particle Method* for solving *Initial-Boundary Value Problems* of partial differential equations authored by J.-S. Chen, W.K. Liu, M.C. Hillman, S.-W. Chi, Y. Lian, and M.A. Bessa. The authors show efficient applications to complex material deformation processes, such as damage softening and failure approximations. Several difficulties exist within these meshfree approximations, such as the necessity of approximate fulfilling Dirichlet Boundary Conditions and especially the necessary accuracy control of numerical integration errors and in consequence the problem of consistent upper bound a posteriori error estimators as the basis for optimal adaptive meshfree refinements. These problems were solved theoretically and numerically in the habilitation thesis of Dr.-Ing. habil. Marcus O. Rüter at our institute at the Leibniz University of Hannover in 2017.

A further new theoretical contribution is the important *Mathematical Foundation of FEM-Type Approximations for Elastoplastic Deformations of Solids*, by D. Reddy, treating the crucial questions of existence and uniqueness and the numerical convergence properties for elastoplastic deformations of solids, represented in space and in process

time. A priori and a posteriori error analysis with at least upper bounds properties can be derived as the *Important Basis for Optimal Mesh Adaptivity* and thus for *Verification*.

New types of generalized mesh-based FEMs and BEMs with hierarchical, spectral and wavelet-based local interpolation functions are efficient for advanced engineering problems, e.g. the so-called FE^2 for multiscale FEMs based on energy balances, further XFEMs mostly used for crack propagation.

Important extensions of classical 1-field FEMs, usually with test and trial functions for displacements, are various types of mixed FEMs, due to Brezzi and Babuška, with the necessity of global inf-sup conditions for guaranteeing numerical stability of global algebraic equation systems. According to the underlying stationarity principle – not an extremum principle – a posteriori error estimators for optimal adaptive mesh refinements require special efforts. A noteworthy new variant is the so-called *Virtual Element Method*.
A remarkable sophisticated mixed method is the *Exterior Calculus* by D. Arnold et al, restricted at the time to the Hilbert Metric and Hilbert and Hodge simplexes for solving second-order elliptic PDEs, systematically worked out in the *Periodic Tables of the Finite Elements* for 2D and 3D element shapes (for triangles, squares, tetrahedrons, cubes, and octahedrons). The crucial advantage in contrast to the Brezzi-type mixed FEM is global numerical stability of the algebraic systems without explicit inf-sup conditions i.e. guaranteeing local numerical stability on the element level.

An essential new chapter treats *Predictive Computational Science: Computer Predictions in the Presence of Uncertainties* by J.T. Oden, I. Babuška, D. Faghili. Major topics are *Mathematical Model Selections, of Statistics of Calibrations, Stochastic Verifications, and the Validation of Models*. Probabilistic and stochastic theories and solution methods are discussed in the chapter *Uncertainty Quantification and Basyian Inversion* by H.G. Matthies.

From the current worldwide experience about the safety reserves of engineering structures, especially steel and pre-stressed concrete bridges with an age of over 30 years, local damages and progressing micro-cracks can be observed worldwide. This is mainly caused by today's much higher and more frequent loads and also by insufficient experimental and theoretical and computational knowledge at the time. Many effects and processes of micro-damage and failure, combined with phase transformations and instabilities at micro-scales in mono- and polycrystalline metal materials, concrete-type brittle materials with the evolution of micro-voids, require sophisticated research for getting reliable information on low- and high-cycle fatigue, aging and various material instability phenomena. Therefore, damage and failure is one of the major research fields worldwide, also for determining inspection intervals and damage tolerances until required structural repairs or improvements.

I amend the concept of a new damage theory for solid materials, based on true analysis of the onset and progression of various damage processes at discontinuous microscales, which I lectured at the COMPLAS conference 2017 in Barcelona, but did not include in ECM2. Classical damage mechanics are based on the simple volumetric Kachanov-Model, and especially the thermodynamic continuum-damage models by the French school were applied since the 1980s, using homogenizations of the discontinuous micro-damage processes at the – mostly discontinuous and anisotropic – micro-scales of materials back to the *Riemann Metric,* related to Riemannian Manifolds, of the C^1 continuous Boltzmann continuum of classical solid mechanics, which does not allow singularities but which are present at the micro-scales. Due to this, the theoretical and numerical results of homogenized damage mechanics cannot truly describe many micro-mechanical onsets and progressions of damage. What we need are molecular kinetics for crystalline materials,

significant for scales of about 1mm and some additional intermediate scales, e.g. based on metrics in Hausdorf Spaces, requiring intermediate mappings in the frame of FE^2 methods.

ECM2 also deals with the important historical stages of development of FEM in computational mechanics after the first mathematical article by R. Courant in 1943 and the engineering article by R.W. Clough et al, followed by a nearly incalculable amount of variants and extensions with applications to all engineering problems. The second phase from about 1976 to about 1990 was characterized by rigorous amounts of Ritz-Galerkin methods with trial and test functions in Sobolev Spaces within finite subdomains, accompanied by a priori and a posteriori error analysis of FEMs and BEMs as the basis for mesh adaptivity. Parallel to this sophisticated engineering modelling took place for complicated linear and non-linear problems. According to the growing computer power and memory and the size and complexity of the engineering problems, efficient commercial software systems were developed and new sophisticated solution algorithms for linear and nonlinear algebraic equations systems for solving millions of unknown variables became necessary.

Further developments require the important properties of the *Methodical Width and Depth* of new theories, numerical methods, and computer programs. *Width* needs simple logical and algorithmic structures and the possibility of extensions to large scales including higher dimensions, thus forming the frame of a box-type structure of computer programs. Methodical *Depth* concerns the extensibility of methods, algorithms, and computer programs to more complicated, e.g. geometrically and physically nonlinear and coupled, problems. This also holds for the implementation of sensitivity analysis for optimization problems. A major task is the definition of parameters for geometrical data, especially for structural optimization processes, at the deepest level, above geometric representation, and uppermost structural data of systems and materials.

Concerning future developments, new physical and mathematical models for the analysis of damage, fatigue and failure are expected, using several adequate metrics in between, from about 1mm to 5mm scales with the molecular kinetic analysis at the lowest scale – e.g. in Hausdorf Spaces – for more accurate descriptions of deformations, damage and fractures at microscales, i.e. apart from the singularity-free Riemann-Metric which is suitable for the macro-scale only. This has to be accompanied by new mathematical theories and their validation.

Additive manufacturing with 3D printing techniques will play an important role in the future, especially in the high-tech areas. This allows for new concepts of designing and producing composite structures based on various material topologies and their distribution and concentration.

The new developments in high-tech industrial products in conjunction with the digital revolution require both box-type and hierarchical concepts for scalable mathematical modelling and computer algorithms for numerical computations.

Chemical Reaction Dynamics: Recent Advances and New Insights

by Kopin Liu, Member EUAS

Short Biography

Education and Positions

2002- Distinguished Research Fellow, Academia Sinica, Taiwan.
2001-2004 Director, IAMS, Academia Sinica, Taiwan.
1993-2001 Research Fellow, IAMS, Academia Sinica, Taiwan.
1982-1993 Staff Scientist, Argonne National Laboratory, IL, USA.
1981-1982 Research Scientist II, Experimental Engineering Station, Georgia Institute of Technology, GA, USA.
1979-1981 Postdoctor, University of Minnesota, Minneapolis, MN, USA.
1977-1979 Postdoctor, University of Toronto, Toronto, Canada.
1973-1977 Ph.D., Ohio State University, Columbus, OH, USA.
1967-1971 B.S., National Tsing Hua University, Hsinchu, Taiwan.

Awards and Honors

Member, EU Academy of Sciences (EUAS), elected 2018.
Richard B. Bernstein Award, XV International Stereodynamics Conference, 2014.
Professor Chau-Ting Chang Memorial Lectureship Award, 2014.
XXV International Symposium on Molecular Beams Award, 2013.
Fellow, The Royal Society of Chemistry (RSC) UK, elected 2013.
CUSO (Conférence Universitaire de Suisse Occidentale) Lecturer, Switzerland, 2012.
Humboldt Research Award, Alexander von Humboldt Foundation, Germany, 2011.
Honorary Chair Professor, National Tsing Hua University, Taiwan, 2010-2012.
Fifty Scientific Achievements, NSC, Taiwan, 2010.
NSC-NRC (Canada) Eminent Researchers Award, 2009-2010.
AS Investigator Award, Academia Sinica, 2008-2012; 2014-2018.
Fellow, The World Academy of Sciences (TWAS), elected 2005.
Academician, Academia Sinica, Taiwan, 2004.
Distinguished Alumni, National Tsing Hua University, 2002.
Distinguished Alumni, College of Science, National Tsing Hua University, 2002.
The Inaugural Presidential Science Prize of Taiwan, 2001.
Fellow, American Physical Society (APS), elected 1998.
Fellow, Foundation for the Advancement of Outstanding Scholarship, 1996-2006.
Chair Scholar, Lin Jun-San Foundation, 1993-1996.

Professional Services

Associate Editor: Chemical Science, 2010-present; Chinese J. of Chemical Physics, 2001-

present; Advanced Series in Physical Chemistry, 2002-2005; J. of Chinese Chemical Society, 2000-2006,
Advisory Board: International Reviews in Physical Chemistry, 2002-present; J. of Physical Chemistry, 2005-2007; J. of Chemical Physics, 2006-2008.
Organizer or co-organizers of 20 International Conferences.

1. Overview

The central theme of my research interests is to gain an in-depth understanding of the fundamental factors that govern chemical reactivity. The experimental work is built around a unique rotatable-sources, crossed molecular-beam apparatus in pioneering the state-to-state scattering measurements under the single-collision conditions—the "Holy Grail" in the field of chemical reaction dynamics. Two new techniques that we developed, the Doppler-selected time-of-flight technique in 1996 [1] and the time-sliced velocity imaging technique in 2003 [2], have proven to be extremely powerful and versatile for studying bimolecular collisions ranging from the prototypical A + BC to more complex polyatomic reactions. The key idea behind both techniques is to project the desired product three-dimensional velocity distribution in the center-of-mass frame directly onto the detector. By exploiting these two innovative approaches, we have not only addressed a number of outstanding scientific issues in chemical dynamics, such as reactive resonances, mode- and bond-selective chemistry, and stereo-specific reactivity, but also uncovered some serious deficiencies in our fundamental understanding of several textbook examples of elementary chemical reactions. Highlighted below are some of the most notable research accomplishments.

2. Reactive or Quantum Dynamic Resonances

Broadly speaking, the term "reactive resonance" refers to a transiently formed short-lived species, or quasi-bound state, produced as the reaction occurs. It is a quantum phenomenon and its existence on a purely repulsive potential energy surface was proposed in the approximate theoretical studies in the early 1970s [3, 4]. This phenomenon has since intrigued physical chemists for many years and it was not clear if it is a genuine phenomenon or an artifact from the theoretical approximations. In 2000 we provided the first unequivocal experimental evidence for a quantum dynamical resonance in the F + HD reaction [5, 6]. That study settled the long-standing controversy ever since the 1985 landmark experiments by Y. T. Lee and coworkers [7, 8] and resolved a 30 year's old mystery in the field of reaction dynamics [9].

Afterwards, we further explored the experimental signatures for reactive resonances in more complex polyatomic systems, such as the reactions of methane (and isotopologues) with F- and Cl-atoms—the possibility that has hitherto never been considered in the literatures [10-12]. These studies offered us the unique opportunity to uncover the intricate intramolecular vibrational dynamics of the transient resonance complex in the transition state region of a reaction [13].

3. Product Pair Correlation

Application of spectroscopic techniques in the study of chemical dynamics provides rich information on the quantum state distributions of the detected products. This conventional method, however, can only reveal the dynamical attributes for one product at the time. More than often, two molecular species are produced in a chemical reaction and the two are formed as a pair. Clearly, merely measuring the outcome of one product is blind to the dynamic attributes of the concomitantly formed coproduct. In 2003 we

introduced the concept of the "product pair-correlation" — a joint probability distribution of the internal states of the two coincidently formed products in a single bimolecular collision event, and devised an experimental method to realize such concept [14]. This ground-breaking work has opened up a completely uncharted territory waiting to be explored and marked a new chapter in the field of chemical dynamics [15].

4. Mode- and Bond-Selective Bimolecular Reactions

How the reactant vibrational mode- or bond-excitation affects chemical reactivity is at the heart of polyatomic reaction dynamics. Using an IR laser to prepare the vibrationally excited reactants, we elucidated the nature of mode-specific and bond-selective chemistry through product pair-correlation measurement, which not only enabled us to gain unparalleled insights into the effects of vibrational excitation on chemical reactivity [16-18], but also led to a conceptual framework for a heuristic view of the cooperative motion of all atoms in the elusive transition-state region [19].

5. Reaction Dynamics beyond the Conventional Transition-State Theory

In an early study of a simple Cl + HD reaction, we discovered unexpectedly the branching ratio of the two isotopic product channels, HCl versus DCl, is dictated by the van der Waals interaction in the entrance valley of the reaction path [20]. More recently, highlighted in a series of studies on the reactions of ro-vibrationally excited CH_4 and CHD_3 with Cl [16], F [17], and $O(^3P)$ atoms [18], compelling evidence were also uncovered for the prominent role of weak long-range interactions in governing the chemical reactivity. These discoveries overturned the conventional wisdom based on the textbook transition-state theory [21, 22]. And a new concept of a passive-control (governed by the intermolecular interactions, as in the reactions of F and $O(^3P)$ with methane) or an active control (manipulated externally by an experimentalist, as in Cl + methane) of chemical reactivity was introduced and elucidated [23].

6. Stereo-Specific Requirement in Chemical Reactions

By taking advantage of our sources-rotatable machine and by exploiting the polarization of IR laser, we pioneered an innovative experimental protocol [24] that enables us to directly visualize the angular correlation between the initial attack angle and the product recoil angle, thus quantitatively delineating the most favorable reaction geometry (or the stereo-specificity of transition state) for the first time in the 40 years' history of stereodynamics of reactions [25-27].

More recently, an entirely new experimental approach was proposed to directly map out the angle-dependent barrier to reaction using polarized scattering data [28]. The result has been validated by a high level *ab initio* calculated potential energy surface. This work represents the first experimental mapping, directly and without resorting to any nuclear dynamics simulation of the experimental observables, of the intermolecular anisotropic interactions in the vicinity of the transition state region. More significantly, the demonstrated scheme is believed to be generally applicable to numerous direct abstraction reactions with a collinear barrier.

References

[1] L.-H. Lai, D.-C. Che, and K. Liu, *J. Phys. Chem.* **100**, 6376 (1996).
[2] J. J. Lin, J. Zhou, W. Shiu, and K. Liu, *Rev. Sci. Instrum.* **74**, 2495 (2003).
[3] S. F. Wu, B. R. Johnson, and R. D. Levine, *Mol. Phys.* **25**, 839 (1973).
[4] G. C. Schatz, J. M. Bowman, and A. Kuppermann, *J. Chem. Phys.* **63**, 674 (1975).

[5] R. T. Skodje, D. Skouteris, D. E. Manolopoulos, S.-H. Lee, F. Dong, and K. Liu, *J. Chem. Phys.* **112**, 4536 (2000).
[6] R. T. Skodje, D. Skouteris, D. E. Manolopoulos, S.-H. Lee, F. Dong, and K. Liu, *Phys. Rev. Lett.* **85**, 1206 (2000).
[7] D. M. Neumark, A. M. Wodtke, G. N. Robinson, C. C. Hayden, and Y. T. Lee, *J. Chem. Phys.* **82**, 3045 (1985).
[8] D. M. Neumark, A. M. Wodtke, G. N. Robinson, C. C. Hayden, K. Shobatake, R. K. Sparks, T. P. Schafer, and Y. T. Lee, *J. Chem. Phys.* **82**, 3067 (1985).
[9] K. Liu, *Annu. Rev. Phys. Chem.* **52**, 139 (2001).
[10] W. Shiu, J. J. Lin, and K. Liu, *Phys. Rev. Lett.* **92**, 103201 (2004).
[11] B. Zhang and K. Liu, *J. Chem. Phys.* **122**, 101102 (2005).
[12] J. Zhou, J. J. Lin, and K. Liu, *Mol. Phys.* **108**, 957 (2010).
[13] K. Liu, *Adv. Chem. Phys.* **149**, 1 (2012).
[14] J. J. Lin, J. Zhou, W. Shiu, and K. Liu, *Science* **300**, 966 (2003).
[15] K. Liu, *Phys. Chem. Chem. Phys.* **9**, 17 (2007).
[16] S. Yan, Y.-T. Wu, B. Zhang, X.-F. Yue, and K. Liu, *Science* **316**, 1723 (2007).
[17] W. Zhang, H. Kawamata, and K. Liu, *Science* **325**, 303 (2009).
[18] F. Wang and K. Liu, *Chem. Sci.* **1**, 126 (2010).
[19] S. Yan, Y.-T. Wu, and K. Liu, *Proc. Natl. Acad. Sci. USA* **105**, 12667 (2008).
[20] D. Skouteris, D. E. Manolopoulos, W. Bian, H.-J. Werner, L.-H. Lai, and K. Liu, *Science* **286**, 1713 (1999).
[21] H. Guo and K. Liu, *Chem. Sci.* **7**, 3992 (2016).
[22] H. Pan, K. Liu, A. Caracciolo, and P. Casavecchia, *Chem. Soc. Rev.* **46**, 7517 (2017).
[23] K. Liu, *J. Chem. Phys.* **142**, 080901 (2015).
[24] F. Wang, J.-S. Lin, and K. Liu, *J. Chem. Phys.* **140**, 084202 (2014).
[25] F. Wang, J.-S. Lin, and K. Liu, *Science* **331**, 900 (2011).
[26] F. Wang, K. Liu, and T. P. Rakitzis, *Nat. Chem.* **4**, 636 (2012).
[27] K. Liu, *Annu. Rev. Phys. Chem.* **67**, 91 (2016).
[28] H. Pan, F. Wang, G. Czako, and K. Liu, *Nat. Chem.* **9**, 1175 (2017).

Recent Trends in Natural Gas Supply Chain Optimization

by Zuo-Jun Max Shen, Member EUAS

Short Biography

Zuo-Jun Max Shen got his PhD from the Department of Industrial Engineering and Management Sciences at Northwestern University. He is now a professor with joint appointment in the Department of Industrial Engineering and Operations Research and the Department of Civil and Environmental Engineering at the University of California, Berkeley. He is also an honorary professor at Tsinghua University and the Co-Director of the Environment and New Energy Center at Tsinghua-Berkeley Institute. He has been active in the following research areas: integrated supply chain design and management, logistics automation and optimization, Energy Systems Optimization, and Transportation System Planning and Optimization, and has overseeing many projects funded by the National Science Foundation, California Department of Transportation and other entities, including the CAREER award from National Science Foundation in 2003. He is currently the senior/area/associate editor for several leading journals in the areas of management science and optimization, such as Management Science, Operations Research, Manufacturing & Service Operations Management, Production and Operations Management, Naval Research Logistics, IIE Transactions, Decision Sciences, and Asia-Pacific Journal of Operational Research. His paper, "A Joint Location-Inventory Model", published in Transportation Science in 2003, was voted one of Transportation Science's most impactful papers in the 50-year history of the journal. His book, Fundamentals of Supply Chain Theory, co-authored with Larry Snyder, won the 2012 IIE/Joint Publishers Book-of-the-Year Award. In 2018, his project on the natural gas supply chain optimization problem faced by China National Petroleum Corporation (CNPC) was selected as one of the finalist teams in the Franz Edelman Award Competition.

As the largest oil and natural gas company, CNPC produced and supplied roughly 70% of domestic natural gas demand last year. In 2014 to 2017, CNPC ranked in the top four of Fortune Global 500.

To help CNPC make better decisions about their pipeline network design and supply chain optimization, we answer the following two questions: first, how much natural gas can be transported by a given network; and second, what is the optimal transmission plan based on the locations of the supply and demand nodes, as well as the different purchasing and sale prices in the network. We address these questions by integrating pipeline natural gas fluid dynamics model into an optimization framework, and jointly optimize natural gas production, import, transmission, storage, and sales decisions.

A precise description of the pipeline model is challenging for two reasons. First, the equations describing the relationship between natural gas flow and pressure involve highly complex nonlinear partial differential equations. For instance, Figure 1 lists four traditional equations for calculating the physical parameters of gas flow dynamics, including the functional forms for specific heat ratio of real gas and temperature adiabatic index, the

Benedict-Webb-Rubin equation for computing the compression factor, and the Joule-Thomson equation for describing gas temperature change. Second, the equations listed in Figure 1 are only applicable when the pipelines are no more than 3 miles long, however a major pipeline can often be as long as 100 miles. It is necessary to divide long pipelines into multiple small ones so that the equations can be directly applied. Consequently, the complexity increases significantly.

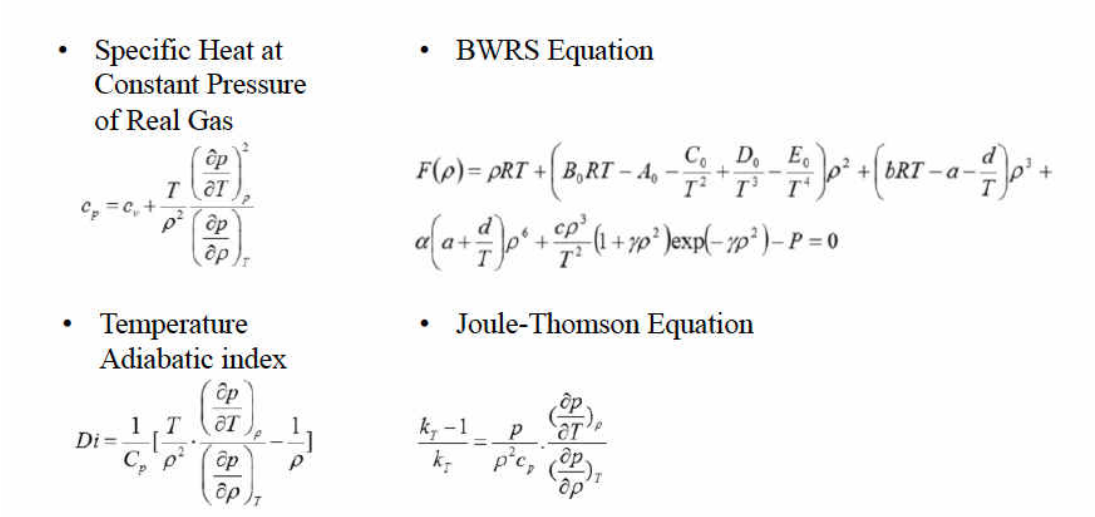


Figure 1. Equations for Parameters in Gas Flow Dynamics

We modeled the natural gas supply chain optimization problem as a nonconvex, non-linear optimization problem. An innovative three-stage solution method was developed to solve large-scale problems efficiently and effectively. In the first stage, the convex relaxed model is solved; in the second, energy minimization model is used to update flow rates; and finally, in the third stage, given flow rates from the second stage, the pressure and temperature are determined.

The successful implementation of the software significantly increased CNPC's profit. In the past three years, CNPC has obtained profit increase of 530 million US dollars during 2015-2017. The increase includes three components. The first component, 340 million US dollars, was from the reallocation of gas selling amounts; the second component, 188 million US dollars, was from the reduction of purchase and transportation costs; and the third component, 2 million US dollars, was from the saving of labor cost.

At the same time, based on the optimal results from the software, CNPC was able to postpone the constructions of 4 main pipelines for 5 years on average, such as the middle part of third west-to-east pipeline. This decision saved roughly 20 billion US dollars of current capital expenditure budget.

This project also has a big environmental benefit in China by giving CNPC more confidence to supply natural gas, which helps alleviate air pollution in China.

References

1. He, L., Mak, H. Y., Rong, Y., & Shen, Z. J. M. (2017). Service region design for urban electric vehicle sharing systems. ***Manufacturing & Service Operations Management*****.** 19(2), pp. 309–327
2. Mak, H. Y., & Shen, Z. J. M. (2016). Integrated Modeling for Location Analysis. ***Foundations and Trends® in Technology, Information and Operations Management*****,** *9*(1–2), 1-152.
3. Lim, M. K., Mak, H. Y., & Shen, Z. J. M. (2016). Agility and proximity considerations in supply chain design. ***Management Science*****.**
4. Qi, W., Liang, Y., & Shen, Z. J. M. (2015). Joint Planning of Energy Storage and Transmission for Wind Energy Generation. ***Operations Research,*** 63(6), 1280-1293.
5. H. Y. Mak, Y. Rong and Z. J. M. Shen (2013). Infrastructure Planning for Electric Vehicles with Battery Swapping. ***Management Science.*** Vol.59, No.7, pp.1557-1575.
6. Atamturk, G. Berenguer and Z.-J. M. Shen (2012). Integer Programming Approach to Stochastic Joint Location-Inventory Problems. ***Operations Research.*** Vol. 60, No.2, pp.366-381.
7. Z. -J. Shen and X. Su (2008). Customer Behavior Modeling in Revenue Management and Auctions: A Review and New Research Opportunities. ***Production and Operations Management***, 16 (6) 713-728.
8. L. V. Snyder and Z. –J. Shen (2006). Managing Disruptions to Supply Chains. ***The Bridge*** (National Academy of Engineering), 36, 4, 39-45.
9. Z. -J. Shen and M. Daskin (2005). Trade-offs Between Customer Service and Cost in Integrated Supply Chain Design. ***M&SOM***, 7, 188-207.
10. Z. –J. Shen (2005). A Multi-commodity Supply Chain Design Problem. ***IIE Transactions***, 37, 753-762.
11. Z.-J. Shen, C. Coullard, M. Daskin (2003). A Joint Location-Inventory Model. ***Transportation Science***, 37, 40-55.
12. M. Daskin, C. Coullard, Z.-J. Shen (2002). An Inventory-Location Model: Formulation, Solution Algorithm and Computational Results. ***Annals of Operations Research*****,** 110, 83-106.

Fatigue Crack Growth Behaviour of Steels in High Pressure Hydrogen

by Ashok Saxena, Member EUAS

Short Biography

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

Dr. Saxena previously held the position of Regents' Professor and Chair of the School of Materials Science and Engineering at the Georgia Institute of Technology in Atlanta and was a Fellow Scientist at the Westinghouse Research and Development Center in Pittsburgh. He also served as the Vice Chancellor of Galgotias University in India for a two year period. As their primary research advisor, he has mentored over 60 MS, doctoral and post-doctoral students.

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

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

Safe and low-cost, high-pressure hydrogen storage systems are a critical need for refueling stations for fuel-cell powered vehicles, for back-up power in buildings, and for fork-lifts in warehouses. Excess energy during high generation periods from renewable sources such as solar and wind can be stored in the form of compressed hydrogen and be made available to power fuel cells during the low generation periods.

Type I, steel pressure vessels constructed from seamless high strength low alloy steel pipes are restricted to maximum pressures of 450 bar. This is due to hardenability considerations that limit the maximum permissible wall thickness of the vessel. Therefore, the challenge is to continue to use steel tanks that have been time-tetsed for storing

hydrogen at about twice the pressure, but limiting the maximum stress in the interior of the vessel via good design to levels that have been successfully used in the past.

Calculations show that the maximum operating pressure of commercially available steel pressure vessels can be approximately doubled by incorporating a hoop wrap using high strength wires with tensile strength of 2 to 4 GPa [1,2]. The wires are held together by epoxy that otherwise does not have a strucrural role. These designs also include subjecting the vessels to hydro-pressures that are about twice the maximum design pressure during manufacturing to produce plastic strains in the liner while maintaining elastic behavior in the high strength steel wire wrap [1,2]. This process is known as autofrettage and the pressure used is called the autofrettage pressure. Upon removal of the autofrettage pressure, compressive stresses are locked into the wall of the steel liner. This, along with effective transfer of stresses from the steel liner on to the wire wrap, reduces the maximum stress in the liner to safe levels.

The American Society for Mechanical Engineers (ASME) has developed codes [3,4] for designing pressure vessels for storing hydrogen but these codes are conservative because of gaps in our ability to confidently model the degradation kinetics of hydrogen embrittlement in these steels. There has been progress in our understanding of mechanisms of hydrogen embrittlement in the crack tip process zone [5] but not sufficient to allow development of robust models for predicting crack growth rates and how they are affected by variables such as loading frequency, load ratios, hydrogen pressure, gaseous impurities, temperature, and material variability. This need has been partially met by empirical studies [6-8]. However, many more such studies must be conducted to meet the overall need of the designers of these vessels. For example, the acceleration of fatigue crack growth rates have been quantified for tension only loading conditions, but autofrettaged pressure vessels experience compression to tension load cycles in service addressed in our research [9].

The experimental results from our studies and those from previously published studies were used to explore the kinetics of environment assisted cracking in A372 Grade J, Class 70 tempered martensitic steels for use in hydrogen storage applications. At 10 MPa H_2 pressure, the FCGR behavior of our test material at a load ratio of 0.2 was compared to the same behavior in air and in helium (He) environment. The results show that the crack growth rates are higher in air than in He and substantially higher in H_2 at 10 MPa. These differences underscore the importance of susceptibility of this material to environment assisted cracking and the need to fully understand it. It is also important to systematically explore the effects of variables such as load ratio, R, loading frequency, ν , and hydrogen pressure on the FCGR behavior.

Effects of Load Ratio

Fatigue crack growth rate tests on single edge crack tension (SEC(T)) specimens, especially designed for testing under fatigue cycles containg negative stresses [10] were conducted under load ratios of -1.0 and -0.5 as well as positive load ratios of 0.1 and 0.2. Positive load ratio data from these tests were compared with data from prior studies [11,12]. Fatigue crack growth rate data obtained on SEC(T) specimens from this study and a from previous study obtained on C(T) specimens appear to be identical at load ratios of 0.1 and a H_2 pressure of 10 MPa. At R = 0.2 our data was at a pressure of 10 MPa while the literature data was at 103 MPa; the FCGR behavior at the higher pressure does show a distinct tendency for higher crack growth rates. The crack growth rates at R=0.5 are higher than the crack growth rates at R=0.1 and 0.2 even after reconciling the differences in pressure.

Comparisons were made between FCGR behaviour at negative load ratios of -0.5 and -

1.0, and the positive load ratios of R=0.1 and 0.2. All data in the current study were generated at a H_2 pressure of 10 MPa. The results show that there is no systematic difference between the FCGR behavior between R values of -0.5 and -1.0. This is entirely expected because negative loads do not contribute to the value of ΔK and if there are any plasticity induced crack closure effects that influence the value of the effective ΔK, they should have saturated for R =-0.5. We note that the R= 0.1 data also blends with the trends for R = -0.5 and -1.0 data. One of the tests at R=0.2 yielded crack growth rates that are very comparable to the rates for R = -1.0, -0.5, and 0.1 while the other showed a somewhat higher rate. This indicates that at R =0.2, the FCGR behavior of A372 Grade J Class 70 steels begins to become sensitive to R in H_2 environment. For R < 0.2, and continuing into negative R values, the FCGR behavior is not sensitive to R even in H_2 environment. For ΔK > 20 MPa$\sqrt{m}$, the differences between air and H_2 are an order of magnitude or more but for ΔK < 10 MPa$\sqrt{m}$, the differences were smaller.

Figure 1 shows a plot of FCGR for values of ΔK of 10, 20, and 30 MPa$\sqrt{m}$ for R values of -1.0, 0.5, 0.1, 0.2, and 0.5. This plot confirms that the dependence of FCGR on R in high pressure H_2 begins to accelerate at R = 0.2. The effects of load ratio in accelerating crack growth behaviour continue even when R increases beyond 0.5 [13]. Also, as mentioned before, the data for R$\leq$ 0.2 was obtained at a H_2 pressure of 10 MPa from this study, and at R =0.5, the test pressure was 103 MPa [11,12]. The da/dN for R =0.5 is higher than for lower load ratios but since it was at higher H_2 pressure, we are unable to separate the effects of R from those due to pressure.

Effects of Loading Frequency

The effect of loading frequency in the range of 10 to 0.001 Hz have been investigated at R =0.1 and H_2 pressures of 10, 45, and 103 MPa for ΔK levels of 15 and 24 MP$\sqrt{m}$. As the loading frequency decreased, the crack growth rates increased modestly. The largest increase in crack growth rates were observed when the loading frequency decreased from 10 Hz to 1 Hz, by approximately a factor of 3. Between 1 Hz and 0.001 Hz, the increase in crack growth rates were small, especially in relation to random scatter in the data. Also, the effects of frequency appeared to be stronger at H_2 pressure of 10 MPa than at 45 and 103 MPa. The results from our studies are shown in Fig.2. These data clearly show only a small effect of frequencies ranging from 1 Hz to 0.01 Hz on the crack growth rates at all ΔK levels.

Effects of Hydrogen Pressure on FCGR Behavior

The effect of H_2 pressure on the fatigue crack growth behavior was investigated by Somerday et al. [17,18]. It is well known that the effects of, load ratio, loading frequency, and pressure can be synergistic so it is impossible to totally isolate the effects of one variable from that of the others [20]. Figure 3 shows the effects of varying H_2 pressure on the FCGR behavior normalized by the rates in air for the same value ΔK for A 372 Grade J, Class 70 steels. Increasing H_2 pressure from 10 MPa to 45 MPa causes an increase in the FCGR by as much as by a factor of 4. But, further increases in FCGR due to increases in pressure from 45 MPa to 100 MPa were small. Differences in crack growth rates due to pressure seem to be smaller for ΔK values in the range of 10 MPa $\sqrt{m}$ than at higher ΔK values of 20 and 25 MPa$\sqrt{m}$. There is evidence that effects of increasing H_2 pressure saturate beyond 45 MPa at the various ΔK levels.

The data show that FCGR behavior in gaseous H_2 do increase with increasing pressure. The magnitude of this effect appears to be highest in going from air environment to 10 MPa H_2 pressure and appears to saturate at 45 MPa level. Additional systematic studies to

accurately quantify the effects of pressure are recommended.

References

1 A. Saxena, A. Prakash, K.A. Nibur, and I. Miller, "Considerations of the Effects of H2 in the Design of Type II Storage Vessels Built for Fatigue Resistance", Proceedings of the International Hydrogen Conference, B.P. Somerday and P. Sofronis editors, ASME-861387, 2017, pp 382-.389.

2 A. Prakash, G.R. Sharp, B.T. Deeken, W.J. Head, W.H. Thomson, "Steel Wrapped Pressure Vessel" US Patent US 9,266,642- B2 issued Feb. 2016.

3 ASME Section VIII, Division 3, Code 2004 Edition, "Alternate Rules for Construction of High Pressure Vessels", ASME New York 10010.

4 M.D. Rana, G.B. Rawls, J.R. Sims, E. Upitis, "Technical Basis and Application of New Rules on Fracture Control of High Pressure Hydrogen Vessel in ASME Section VIII Division 3, PVP 2007-2603, 2007, ASME PVP Conference, San Antonio, Texas.

5 R.P. Gangloff "H2-Enhanced Deformation and Fracture in the Crack Tip Plastic Zone", Proceedings of the International Hydrogen Conference, B.P. Somerday and P. Sofronis editors, ASME-861387, 2017, pp.1-35.

6 K.A. Nibur, and B.P. Somerday, "Fracture and Fatigue Test Methods in Hydrogen Gas" Gaseous Hydrogen Embrittlement of Materials in Energy Technologies, R.P. Gangloff and B.P. Somderday, eds., Woodhead Publishing Ltd., Cambridge, Vol. 1, 2012, pp.195-236.

7 B.P. Somerday, P. Bortot, and J. Felbaum, "Optimizing Measurement of Fatigue Crack Growth Relationships for Cr-Mo Pressure Vessel Steels in Hydrogen Gas", PVP2015-45424, Proc. ASME PVP Conference, July 19-23, 2015, Boston, MA.

8 K. A. Nibur, B.P. Somerday, C. San Marchi, J.W. Foulk, M. Dadfarina, P. Sofronis, "The Relationship Between Crack Tip Strain and Subcritical Cracking Thresholds in Steels in High Pressure Hydrogen Gas" Met. Transactions A, Vol. 44, 2013, pp248-269.

9 A. Saxena, K.A. Nibur, and A. Prakash, "Applications of Fracture Mechanics in Assessing Integrity of Hydrogen Storage Systems" Engineering Fracture Mechanics, 187, 2018, pp 368-380.

10 A. Saxena, F. Bassi, K.A. Nibur, and J.C. Newman, Jr., "On Single-Edge-Crack Specimen Tension-Compression Fatigue Crack Growth Testing", Engineering Fracture Mechanics, 176, 2017, pp 343-350.

11 B. P. Someday, P. Berlot, J. Felbaum, "Optimizing Measurement of Fatigue Crack Growth Relationships for Cr-Mo Pressure Vessel Steels in Hydrogen Gas", PVP-2015-45424, Proceedings of the ASME 2015 Pressure Vessel and the Piping Division Conference, July 19-23, 2015, Boston, MA

12 B.P. Somerday, C. San Marchi, and K. A. Nibur, "Measurement of Fatigue Crack Growth Rates in SA372 Grade J Steel in 100 MPA Hydrogen Gas Following Article KD-10, PVP 3013-97455, Proceedings of ASME 2013 Pressure Vessel and the Piping Division Conference, July 14-28, 2013, Paris, France.

13 San Marchi, C., Bortot, P., Felbaum, J., Wada, Y. and Ronevich, J.A. "Fatigue and Fracture of High-Hardenability Steels for Thick-walled Hydrogen Pressure Vessels" Proceedings of the International Conference on hydrogen Safety, Sept 11-13, 2017, Hamburg Germany.

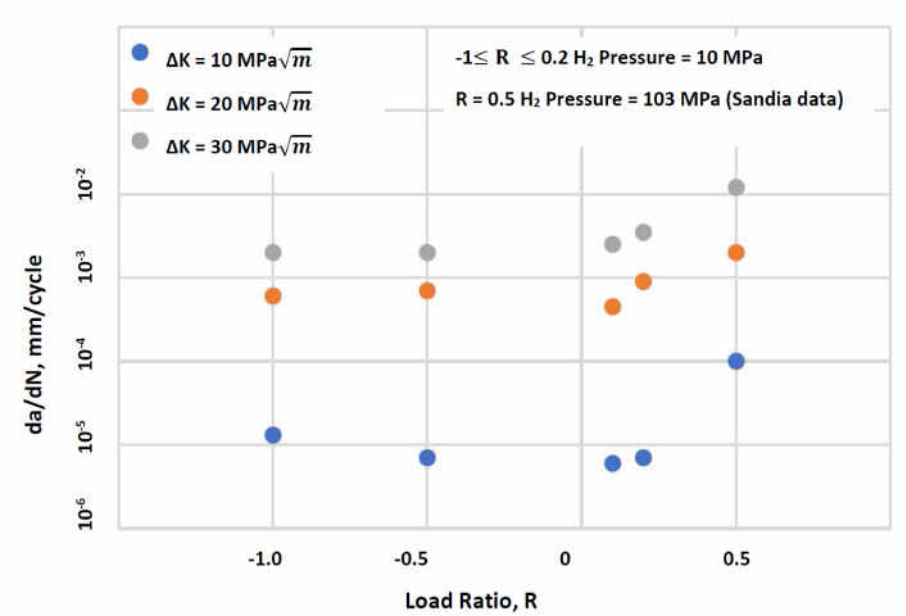


Fig. 1- FCGR behavior of A372 Grade L Class 70 as a function of load ratio R for three values of ΔK

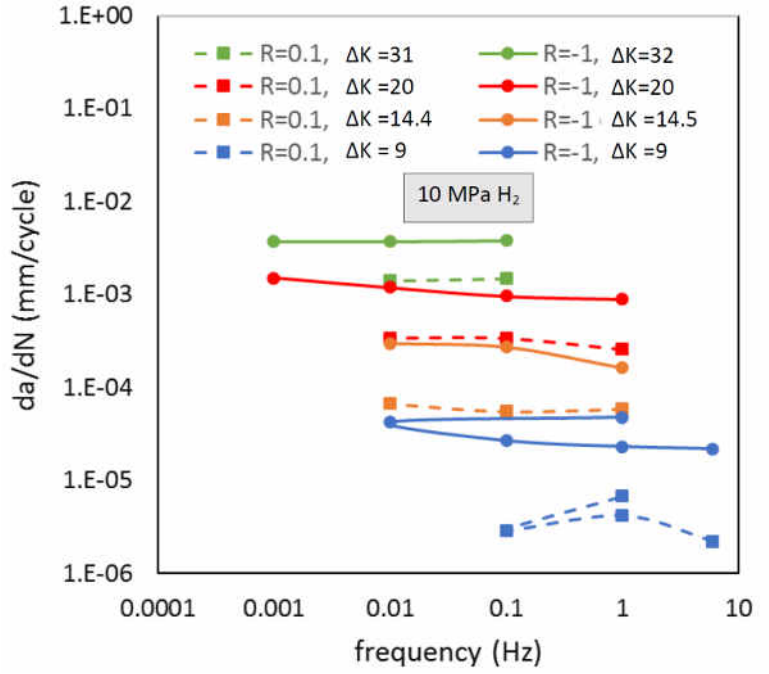


Fig. 2- Effect of loading frequency on the fatigue crack growth rates in 10 MPa H_2 pressure at R = -1.0 and at R = 0.1 at four ΔK levels for A372 Grade J Class 70 steel.

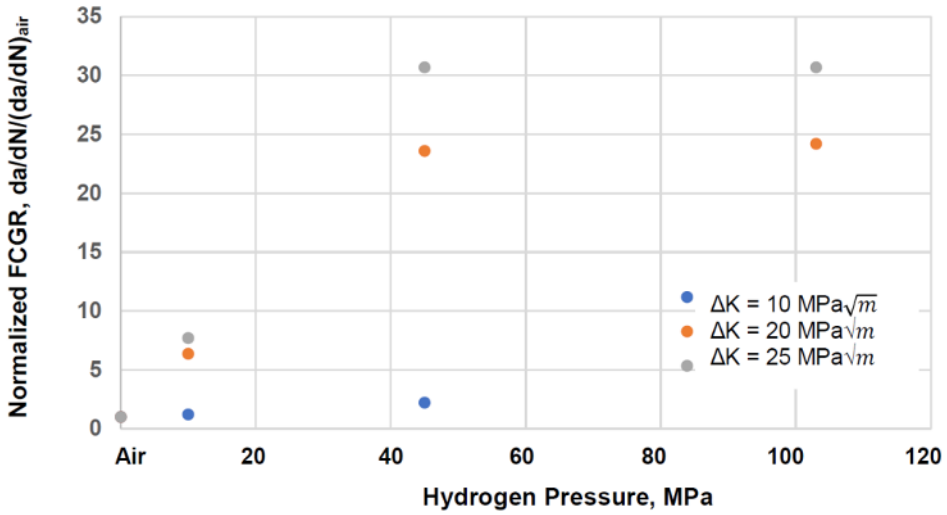


Fig. 3- FCGR behavior in H_2 gas environment at various pressures normalized by the corresponding crack growth rates in air to highlight the extent of embrittlement.

Overview on CBS Extrapolation and its Implications

by Antonio Varandas, Member EUAS

Short Biography

A.J.C. Varandas received a diploma in Chemical Engineering from the University of Oporto (Portugal), and a Ph.D. in Theoretical Chemistry from the University of Sussex (U.K.) under the direction of Professor John N. Murrell.

After graduation in Oporto, he joined the staff at the Department of Chemistry of the University of Coimbra as Assistant Professor, where he occupies since 1988 a position of Full Professor and directs the group of Theoretical & Computational Chemistry. In 1988, he was Invited Professor and Visiting Research Scholar of Minneapolis Supercomputer Institute at the University of Minneapolis (USA) and, from June-July 1995, Cherry L. Emerson Fellow at the Department of Chemistry of Emory University in Atlanta (USA).

In 2009, he was awarded a Visiting Professorship for Senior International Scientists from the Chinese Academy of Sciences. His research interests cover a wide range of topics in theoretical chemistry from potential energy surfaces to non-adiabatic effects in ro-vibrational spectroscopy and reaction dynamics. Some of his studies have implications on theoretical environmental chemistry, particularly in combustion chemistry and issues related to the ozone chemistry at the middle atmosphere.

He has 400 research papers in those areas, and co-authored a monograph entitled Molecular Potential Energy Functions (Wiley, 1984). Edited special issues of Physica Scripta (IOP, 2011), and Advances in Physical Chemistry (Hindawi, 2012), and co-edited a book in memorial of Ruy Couceiro da Costa (Universidade de Coimbra, 2011). Wrote 2 books and 2 books of lectures notes, all in portuguese, devoted to Computational Methods, Quantum Chem-istry, and Statistical Mechanics.

Oriented 30 PhD students from various nationalities, including Brazil, China, Cuba, India, Italy, Moldavia, Portugal, and Spain. Received the following awards: "Artur Malheiros" Prize for Physics and Chemistry of the Lisbon Academy of Sciences (1985); "Ferreira da Silva" Prize of the Portuguese Chemical Society (1991); Prize Stimulus to Excellence of the Portuguese Ministry of Science, Innovation and High Studies (2004).

Received honorific titles from Insituto Superior de Tecnologias y Ciencias Aplicadas (La Habana, Cuba, 1998), Dalian Institute of Chemical Physics (Dalian, China, 2005), and Henan Normal University (Henan, China, 2006). In 2006, he was elected corresponding member of the Lisbon Academy of Sciences. Also, in 2015 he was elected member of the EU Academy of Sciences.

The problem of extrapolating the energy to the complete one-electron basis-set limit in ab initio electronic structure calculations is overviewed. Only the correlation energy is considered in detail since it is the most difficult to converge. With the uniform-singlet-and-triplet-extrapolation (USTE) scheme at the focal point, the emphasis is on recent updates. Some implications and prospects for future work conclude the overview.

Introduction

Approximations are unavoidable in molecular physics, with the Born-Oppenheimer (BO) approximation being most fundamental. Owing to mass disparity (nuclei are 1837 times heavier than electrons), BO proposed that the motions of nuclei and electrons could be treated separately: the former are said to move adiabatically on by the potential energy surface (PES) created by the latter. As a result, the electronuclear Schrödinger equation splits into two: one for electrons moving in a fixed arrangement of the nuclei (electronic Schrödinger equation, eSE), the other (nSE) for nuclei moving on the electronic PES. Only the former is of concern in the present work

Two major difficulties (or "explosions") characterize computational quantum chemistry: a) the $\mathcal{X}^{3N-6}$ explos-ion estimates the number of times that the eSE needs to be solved to map a N-atom PES ($\mathcal{X}$ is the number typically required/dimension); b) the $\mathcal{X}^{12}$ explosion shows how the cost/point raises with the basis set cardinal number $\mathcal{X}$.[2] Added to them is the need for PESs with chemical accuracy (< 1 kcal mol^{-1}) in reaction dynamics, and spectroscopic acc uracy (< 1 cm^{-1}) if rovibrational calculations are at stake. Both imply a PES at the one-electron complete basis set (CBS) level. Extrapolation methods are then required. Embedding no empiricism, they may be at a pure mathematical level (using polynomials and rational fractions) or use a physically motivated asymptotic theory as is here the case.

Theory

Methods for solving the eSE have long been of utmost importance in computational molecular science. The simplest is Hartree-Fock (HF), a mean-field theory where electron correlation is ignored. The error due to its disregard is significant giving way to more sophisticated single-reference (SR) MO-based ones: variational (com-figuration interaction, CI), perturbative Møller-Plesset (many-body perturbation theory, e.g., MP2), and couple-cluster (CC). Of these, the CC singles and doubles with perturbative triples method, CCSD(T), is commonly viewed as the golden rule of quantum chemists. Of course, SR methods still miss the nondynamical cor-relation, which is recovered at the multireference (MR) level. Because integration of the eSE with accuracy at demand is unreachable, extrapolation of the calculated raw energies is key and the focal point here.

The electron-electron repulsion operator is singular at r_{12}=0, and hence the exact wave function must show a discontinuous derivative as implied by Kato's cusp condition. Conventional methods fail to satisfy the latter, which explains their very slow convergence. Although the purist way to solve the problem would be to make the many-electron wave function depend explicitly on $\mathbf{r}_{12}$, the alternative is to systematize the error of conventional methods and extrapolate to predict the inherent error.

From a partial-wave expansion for two-electron atoms, it has been established that: a) for natural-parity singlet states, the leading contribution to the energy at second-order of perturbation theory is $\propto(\ell+1/2)^{-4}$ with no odd-terms either $\propto(\ell+1/2)^{-5}$ or $\propto(\ell+1/2)^{-7}$; b) for triplet states, the leading term is $\propto(\ell+1/2)^{-6}$. Such findings remain essentially unaltered for atoms with any number of electrons. If $\Delta E_l \propto \sum_{m=4} a_m(l+1/2)^{-m}$, the convergence error when all $l \geq L$ terms assumes the form:

$$\Delta E = \sum_{l}^{\infty} \Delta E_l \sim \sum_{m=4} a_m \int_{L+\frac{1}{2}}^{\infty} \left(l+\frac{1}{2}\right)^{-m} dl$$
$$= \sum_{m=4} A_{m-1}(L+1)^{-m+1} \quad (1)$$

with $A_3(L+1)^{-3}$ and $A_5(L+1)^{-5}$ being the first two leading asymptotic terms. As recently noted, considering just the first term can be accuracy-limiting.

Largely motivated by the above, modern basis sets are commonly built according to a principal expansion. Examples are the popular correlation-consistent basis sets (cc-pV*X*Z or V*X*Z, etc) where the cardinal number *X* (=2:*D*, 3:*T*, 4:*Q* ...) is identifiable with *L*+1. Such a slow convergence compounds with the further scalings of MP2, CCSD, and CCSD(T), in this order $N^5N_b^4$, $N^6N_b^4$, and $N^7N_b^4$, where N_b is the number of basis functions per atom; $N_b \simeq X^3$ for a V*X*Z basis. Because correlated calculations beyond *QZ* are unaffordable for many interesting systems, the raw energies are left too far for a safe extrapolation. Since the focal point here is the cor-relation energy, suffice to add that the HF energy con-verges exponentially, while being also computationally less demanding.

The USTE Scheme: Update 2018

Despite a fast convergence (often reported $\propto X^{-7}$), explictly correlated (R12-type) methods appear to perorm inefficiently with small basis sets. CBS extrapol-ation of conventional electronic energies is best per-formed by first splitting the total energy into its HF and correlation components. The latter varies $\propto X^{-3}$ for opposite spin electron pairs and $\propto X^{-5}$ for pairs with the same spin. The USTE scheme accounts for both as:

$$E_X^{\rm cor} = E_\infty^{\rm cor} + \frac{A_3}{(X+\alpha)^3}\left[1+\frac{\tau_{53}}{(X+\alpha)^2}\right] \quad (2)$$

where $\tau_{53} = (A_5^o/A_3) + cA_3^{m-1}$; α, A_5^o, and c are "universal" *ab-initio*-based parameters. Empirical-free and with the correct asymptotic behavior, it is a dual-level scheme that gives a prediction as accurate as one possible can get when extrapolating from raw energies for the two highest affordable *X* values. Yet, a scheme using at most (*D, T*) is key for larger systems. This is the goal of GUSTE, where τ_{53} is suggested to be invariant over configuration space once determined for one geometry with $X \geq$ Q raw data. Clearly, even this is out of reach for large molecules.

Eq. (2) may also be rewritten as:

$$E_X^{\rm cor} = E_\infty^{\rm cor} + \frac{A_3}{\tilde{X}^3} \quad (3)$$

where the hierarchical number $x = \tilde{X}$ is defined by:

$$\tilde{X} = (X+\alpha)\left[1+\frac{A_5/A_3}{(X+\alpha)^2}\right]^{-1/3} \quad (4)$$

The novel concept is that the basis is "educated" to account for deficiencies on its composition according to the recovered correlation energy. Stated differently, a hierarchical staircase as straight as possible in X^{-3} is envisaged to enhance reliability when extrapolating from any two steps. Although more than one possibility exists for the reassignment, we suggested to obtain the new hierarchical numbers as statistical averages of the values obtained from the condition that the $X \lessapprox 6$ values fall on the straight line obtained by fitting USTE(5,6) correlation energies. The method maintained the same acronym but specifying the hierarchical number-pair used for the extrapolation: USTE(x_1, x_2). The novel hier-archical numbers x=d, t, q, p, h ... are real positive but still universal as they apply equally well to any correlation-consistent-type basis sets. Since the correspondence for subminimal [sM, thence smaller than *DZ* or minimal (M); larger than these are named extended (E)] basis sets may not be obvious, the bases may alternatively be indicated.

Finally, Figure 1 compares our CBS extrapolated correlation energies with the best available results.

Conclusions

Saturating a basis to achieve chemical accuracy in electronic structure calculations is key but unaffordable for medium- and large-sized molecules. CBS extrapolation offers a cost-effective and reliable way out, and we have shown how to obtain highly cost-effective but reliable correlation energies from extrapolation with (sM, N) basis set pairs. This has been possible due to a novel USTE$_a$ scheme that allows to hierarchize any available basis sets from the recovered correlation energy. Because the joint use of a SM and an E basis costs nearly as much as a single-point with the latter, USTE$_a$ has become as efficient and perhaps even more reliable than any genuine single-level scheme despite being dual-level. Extrapolation of the HF energy is also key, a subject that has been dealt with elsewhere. Due to the low-cost and reliability of MP2/CBS(sM, M) and MP2/CBS(M, M) methods *vs* KS DFT, a wealth of topics may become open to revisitation, ranging from CBS extrapolations in large systems to explicitly correlated calculations and on-the-fly dynamics. And this may even become doable with Sturmian functions of which Slater-type orbitals are a particular case. Per se or jointly with cost-free MP2-VOS theory, the novel developments may be expected to have a broad impact in chemistry and materials science.

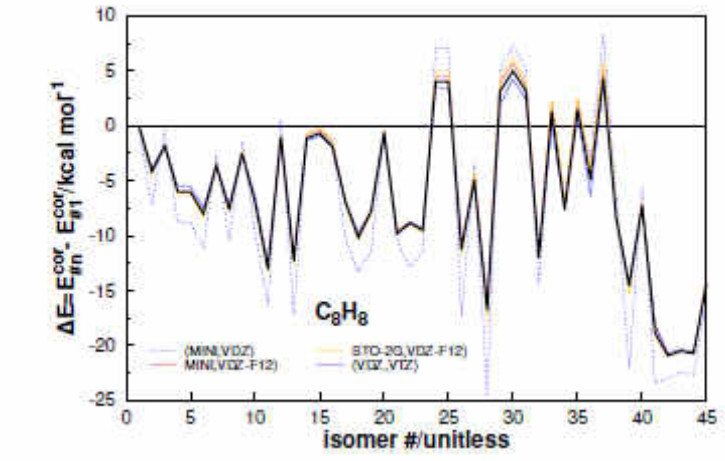


Figure 1: Energy separations of the C_8H_8 isomers at CCSD(T) level of theory; see elsewhere for their names and B3LYP geometries. Shown in solid black is CBS(VDZ-F12, VTZ-F12).