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ABSTRACT BOOK

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Plenary Presentation

A Physico-Chemical View on Redox-Based Memristive Switching in Metal Oxides

Rainer Waser[1,2*]
Regina Dittmann[1]
Stephan Menzel[1]

[1]JARA-FIT & PGI-7, Forschungszentrum Jülich, 52425 Jülich
[2]IWE2, RWTH Aachen University, 52056 Aachen

Abstract

Redox-Based Resistive Switching Memories (ReRAM), also called nanoionic memories or memristive elements, are widely considered to provide a potential improvement beyond the limits of current memory technology with respect to write speed, write energies, and scalability as well as an energy-efficient approach to neuromorphic computing concepts.

In this talk, fundamental aspects of the physics and chemistry (lattice disorder, ionic and electronic transport processes, and phase formation) of these elements will be presented. In particular, the polarity of the switching (eightwise or counter-eightwise) and the geometry (conducting filament vs. area dependent switching) will be discussed. Furthermore, the ultra-high non-linearity of the switching kinetics of redox-based resistive switching devices will be outlined with an emphasis on the so-called valence change mechanism (VCM) typically encountered as a bipolar switching in metal oxides, but also mentioning the electrochemical metallization (ECM) cells. The involved electrochemical and physical processes can be either electric field/voltage enhanced or accelerated by a local increase in temperature due to Joule heating

The two major strands of neuromorphic computing, namely the computational neuroscience for decoding the human brain and artificial neural networks for pattern recognition, will be worked out. And the different requirements on memristive elements to be applied in these two strands will be discussed.

Biography:

Rainer Waser received his PhD in physical chemistry at the University of Darmstadt in 1984, and worked at the Philips Research Laboratory, Aachen, until he was appointed Professor at the faculty for Electrical Engineering and Information Technology of the RWTH Aachen University in 1992 and director of the Institute for Electronic Materials at the Forschungszentrum Jülich, in 1997. Together with Professor Wuttig, he heads a collaborative research center on resistively switching chalcogenides for future electronics (SFB 917) since 2011. In 2014, Rainer Waser received the Leibniz Prize of the DFG for his work on the phenomenon of redox-based resistive switching.

Keynote Presentations

Light-Biological Matter Interaction and Potential Clinical Utilities

Zirui Liu[1]
Tieyi Li[1]
Zeyu Wang[2]
Yong Kim[3]
Shan Huang[1]
Jun Liu[1]
Byoung Hoon Min[4]
Ji Young An[4]
Kyoung Mee Kim[5]
Sung Kim[6]
Yiqing Chen[7]
Huinan Liu[7]
David T.W. Wong[3]
Tony Jun Huang[2]
Ya-Hong Xie1*

[1]Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, CA 90095, USA
[2]Department of Mechanical Engineering and Material Science, Duke University, Durham, NC 27708, USA
[3]UCLA School of Dentistry, 10833 Le Conte Ave. Box 951668, Los Angeles, CA 90095-1668, USA
[4]Department of Medicine, Samsung Medical Center, Sungkyunkwan University School of Medicine, Seoul, Korea
[5]Department of Pathology and Translational Genomics, Samsung Medical Center, Sungkyunkwan University School of Medicine, Seoul, Korea
[6]Department of Surgery, Samsung Medical Center, Sungkyunkwan University School of Medicine, Seoul, Korea
[7]Department of Bioengineering, University of California, Riverside, Riverside, CA 92521, USA

Abstract

Light-biological matter interaction holds promise in biosensing with the associated application potential to include disease diagnosis, drug development, and therapeutics. Our research focus on the utility of a physics-based phenomenon known as surface enhanced Raman spectroscopy (SERS). This line of scientific/technological pursuit by several research groups around the world including that of our own uses SERS spectra as biomolecular “fingerprint” to identify the homeostatic state of biological samples such as cells and exosomes with the help of machine learning for pattern recognition. With regard to materials, our research contributes to expanding material characterization to beyond the traditional inorganic materials into the territory of the homeostasis of biological microsystems.

In this talk, I will share our journey from benchmarking the capability of SERS in fingerprinting biological entities to our attempts in using such fingerprints for disease diagnostics. The specific topics of discussion include cancer diagnostics using exosomes, SARS-CoV-2 diagnosis, and the objective diagnosis of Alzheimer’s disease. The success and challenges along these lines of research will be discussed. The physics of SERS together with the primary factors contributing to the spectral features and its quantitative analysis capability will be presented. The primary considerations in selecting appropriate machine learning algorithms will also be discussed. Finally, the prospect of this sensing technology to enter clinical practice and drug development based on the published results of the various research groups across the world including that of our own will be discussed.

Biography:

Ya-Hong Xie is a professor and vice chair of the department of materials science and engineering at the University of California Los Angeles (UCLA). Prior to joining the UCLA faculty in 1999, he spent 14 years at Bell Laboratories conducting research on semiconductor materials and devices. The interests of his group at UCLA include surface plasmon enabled biosensing and the materials and devices of wide bandgap semiconductors. He has over 200 journal publications and holds 38 US patents. He is a fellow of IEEE and a winner of 2012 Research Award of Alexander von Humboldt Foundation.

Plasmonic Materials for Solar Energy Conversion, Biosensing and Photodynamic Cancer Treatment

Nianqiang Wu

Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA 01003-
-9303, USA

Abstract

Materials can harvest light efficiently and store abundant energy using surface plasmon resonance (SPR). This talk presents our studies on transfer of the stored energy to neighboring materials and media for solar energy conversion, biosensing and photodynamic cancer treatment. This talk is focused on the design, energy transfer mechanisms and usage of plasmonic metal-semiconductor heterojunctions and plasmonic metal-biomolecule hybrids.

Biography:

Nianqiang (Nick) Wu is Armstrong-Siadat Endowed Chair Professor in Materials Science in Department of Chemical Engineering at University of Massachusetts Amherst. He is Fellow of the Electrochemical Society (FECS) and Royal Society of Chemistry (FRSC). He received several honors and awards such as Highly Cited Researcher (Clarivate Analytics, Thomson Reuters), ECS Sensor Division Outstanding Achievement Award, Benedum Distinguished Scholar Award, the Alice Hamilton Award for Excellence in Occupational Safety & Health, and George B. Berry Chair of Engineering (WVU). His research interest lies in (i) photocatalysts and photoelectrochemical cells, (ii) electrochemical energy storage, and (iii) biosensing and photodynamic therapy.

Aqueous Auto-Dispersion for Advanced Materials

John Texter*

Coating Research Institute, School of Engineering, Eastern Michigan University, Ypsilanti, MI 48197, USA

Abstract

Free-energy driven dispersion formation is piqued by microscopic to nanoscopic phase separation from macroscopic phases of components exhibiting an intriguing balance of chemical forces. We describe designs and syntheses of examples of such thermodynamically stable nanoparticle dispersions derived by condensation and radical-chain polymerizations. A key attribute of these examples is their incorporation of polymerized ionic liquids (PIL) that also impart stimuli-responsive behaviors to such nanoparticles and dispersions derived from

such nanoparticles. These systems are found to undergo reversible first and second order phase transitions and promise to support development of mesoscale thermodynamics of crystallization, precipitation, crystallization frustration, and multiphase coexistence.

Four example classes of such thermodynamically stable dispersions are illustrated: (1) multiblock copolymers made by controlled emulsion polymerization; (2) polysiloxanes derived by sol-gel processing; (3) polyurethane dispersions2 via condensation step-polymerization; (4) polyester dispersions via condensation polymerization. Some of these examples are room-temperature liquids and all incorporate ionic liquid monomer. They form thermodynamically stable dispersions in water and auto-disperse when contacted with water. This free-energy-driven auto-dispersion (self-dispersion) distinguishes these diverse polymers because of a significant practical consequence of such a characteristic: very-low energy manufacturing (high-shear-free) of 10-30% by weight dispersions.

Their respective ionic liquid components impart diverse stimuli-responsive behaviors. One significant behavior is reversible destabilization-stabilization of respective nanoparticle dispersions. Those that incorporate imidazolium-based ionic liquid monomers are also excellent stabilizing aids for nanocarbons, such as graphene and carbon nanotubes.

Biography

John Texter is Professor Emeritus of Polymer and Coating Technology at Eastern Michigan University and consults through Strider Research Corporation. He received his undergraduate engineering education and his PhD in Chemistry from Lehigh University, where he studied at the Zettlemoyer Center for Surface and Coatings Research. He is an experienced lecturer, technical project manager, inventor, editor, and author of over 250 publications including five books, 47 issued U.S. patents, and many research and review articles. He a Fellow of the American Physical Society, the American Chemical Society, and of the Society for Imaging Science and Technology. . His research focuses on stimuli responsive polymers, particles, and materials and the general area of dispersion science and practice.

Oral Presentations

Structural Origin of Reversible Li Insertion in Guest-Free, Type-II Silicon Clathrates for Applications as Li-ion Battery Anodes

Xihong Peng[1*]
Andrew Dopilka[2]
Candace K. Chan[2]

[1]College of Integrative Sciences and Arts, Arizona State University, Mesa, Arizona 85212

[2]Materials Science and Engineering, School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, Arizona 85827

Abstract

The guest-free, type-II Si clathrate (Si136) is an open cage polymorph of Si with structural features amenable to electrochemical Li storage. However, the detailed mechanism for reversible Li insertion and migration within the vacant cages of Si136 is not established. Herein, X-ray characterization and density functional theory (DFT) calculations are used to understand the structural origin of electrochemical Li insertion into the type-II clathrate structure. At low

Li content, instead of alloying with Si, topotactic Li insertion into the empty cages occurs at ≈ 0.3 V versus Li/Li+ with a capacity of ≈ 231 mAh g−1 (corresponding to composition Li32Si136). A synchrotron powder X-ray diffraction analysis of electrodes after lithiation shows evidence of Li occupation within the Si20 and Si28 cages and a volume expansion of 0.22%, which is corroborated by DFT calculations. Nudged elastic band calculations suggest a low barrier (0.2 eV) for Li migration through interconnected Si28 cages, whereas there is a higher barrier for Li migration into Si20 cages (2.0 eV). However, if Li is present in a neighboring cage, a cooperative migration pathway with a barrier of 0.65 eV is possible. The results show that the type-II Si clathrate displays unique electrochemical properties for potential applications as Li-ion battery anodes.

Reference: Dopilka, A., Weller, J.M., Ovchinnikov, A., Childs, A., Bobev, S., Peng, X. and Chan, C.K. (2021), Adv. Energy Sustainability Res. 2000114. https://doi.org/10.1002/aesr.202000114

Biography:

Xihong Peng is a Professor in College of Integrative Sciences and Arts at Arizona State University (ASU) Polytechnic campus. She received her Ph. D in Physics from Rensselaer Polytechnic Institute, New York, USA, in 2007. She joined ASU in 2008 as an Assistant Professor, and was promoted to an Associate Professor and Professor in 2014, and 2021, respectively. Her research expertise is first-principles density-functional theory calculations on materials to gain a fundamental understanding of the materials' properties at an atomic level.

Polymerization Shrinkage Analysis during Dental Restoration Observed by Digital Image Correlation

Jung-Hoon Park[1]
Nak-Sam Choi[1*]

[1]Hanyang University, South Korea

Abstract

Mechanistic polymerization shrinkage and stress behaviors of two different kinds of dental composite resins (Filtek P90 (3M ESPE, USA), Clearfil AP-X (Kuraray, Japan)) were investigated with digital image correlation (DIC) method using CCD camera during and after light irradiation. For both resins, the interior of the resin part exhibited greater radial shrinkage strain (εr) due to more mobility than the resin margin near the substrate ring, where a non-symmetric distribution of εr was mostly observed with a peak which had been located a bit away from the center.

The average radial shrinkage strain ($\bar{\varepsilon}$r) of the resin in the central region was approximately 3.9 times greater for P90 and 2.1 times greater for AP-X than the marginal region of the resin. After the curing test, the maximum $\bar{\varepsilon}$r appeared around 0.5mm from the center. The absolute radial shrinkage strain decreased from around the center to the margin adhered to the substrate. The percentage of shrinkage progress around the center for P90 during light irradiation was 33% for 90 and 57% for AP-X against the completed shrinkage at the test end, and indicated very different shrinkage rates for the two resins. The first principal strain calculated by the normal and shear strains on the resin surface showed peak values along the margin interface. For both P90 and AP-X, the maximum principal stress converted from the principal strain was thus concentrated in the vicinity of the interface: 3.06 to 16.1 MPa for P90

and 7.44 to 40.2 MPa for AP-X. The maximum principal stresses along the margin were 1.5–8.4 times highly larger for both resins than the corresponding values by FEM. The non-symmetric shrinkage and the large shrinkage rate during light irradiation caused a significant increase in the principal tensile stress along the interface with the substrate.

Biography:

Nak-Sam Choi has been a professor of Department of Mechanical Engineering, Hanyang University (ERICA), Korea since 1995. He received his BS in Mechanical Engineering from Seoul National University, Korea in 1981, his MS in Mechanical Engineering from KAIST, and Ph.D in Composite Materials & Applied Mechanics from Kyushu University, Japan in 1990. His research interests include fatigue life and microstrain analysis, non-destructive examination of advanced materials and composites, and reliability life of mechanical components.

New Design Strategy and Applications for Electrochemically Stable and Processable Polyaniline

Colleen Scott

Mississippi State University, Starkville, MS

Abstract

Derivatives Advancement in the organic device technology relies greatly on the processability, efficiency, and stability of the organic materials that comprise the devices. An in depth understanding of the impact of the chemical structures on the electrochemical processes of redox polymers is of utmost importance to the development of durable redox materials. Polyaniline (PANI) stands out among the many different conducting polymers (CPs), due to its outstanding air and moisture stability, simple preparation technique, high conductivity, and low cost. Only a very few CPs (PANI and PEDOT) have gained some large-scale commercial applications, mostly due to the lack of electrochemical stability and processability of CPs. However, PANI and PEDOT can only be processed by advance dispersion methods, which increases the processing cost. PANI's commercial applications includes printed circuit board manufacturing, antistatic and electrostatic dispersive (ESD) coatings, and corrosion protection. Even so, PANI has great potential for applications in many other fields such as supercapacitors and batteries, electronic devices as holeinjection layers, solar cells, biosensors, and toxic metal recovery. Unfortunately, practical applications of PANI in these fields are limited by the material's electrochemical instability, and the lack of standard deposition methods. These challenges are very difficult to overcome for PANI, and all efforts to improve the electrochemical stability and processability of PANI films have not been able to sufficiently overcome these deficiencies for commercial applications. In this presentation, we discuss our approach towards the development of processable redox PANI-derivatives that are electrochemically stable by using heteroatom and side chain engineering. Phenoxazine, phenothiazine, carbazole, and other heteroatomfused cores are modified and polymerized to obtain PANI-like structures that are shown to be electrochemically stable and easily processable on a large scale due to their high solubility in common organic solvents. The polymers are also highly conductive and possess the usual electrochromic properties; as such, these properties are exploited in applications such as 3D printing of organic devices and stretchable sensors, which we will discuss in our presentation.

Nanoscale Engineering of Oxide Particles for Oxygen Electrocatalysis

Meng Zhou
Hongmei Luo*

Department of Chemical and Materials Engineering, New Mexico State University, NM 88003

Abstract

The global energy crisis coupling with the consumption of fossil fuels and the associated environmental issues, has stimulated extensive interest in searching for clean, efficient and sustainable energy storage and conversion systems. Oxygen electrocatalysis, including both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), dominates the performance of the devices. However, the sluggish kinetics of these two reactions limits their performance. Therefore, development of non-precious metal-based oxygen electrocatalysts, especially with bifunctionality for both OER and ORR, is greatly demanded. Metal oxides have attracted extensive interest as alternative electrocatalysts due to their low price and good endurance under relatively high temperature, which can be doped with a wide range of cations attributed to their flexible compositions and structures, leading to easy manipulation of their electrocatalytic properties. In this talk I am going to introduce a novel chemical solution approach for oxide nanoparticle network synthesis. The use of water soluable polymer to bind the metal ions has several advantages. We study the nanoscale engineering of perovskite oxides and layered oxides in energy conversion/storage devices and focus on the electrode catalyst design and fabrication for boosting electrocatalysis in fuel cell, electrolyzer, and metal-air batteries, especially using our unique polymer-assisted solution method, various strategies (A-site cation deficiency/excess, A-site doping, B-site doping, and co-catalyst) to boost the performance of catalyst activity with reduced materials cost and good durability as well as to gain low total overpotential.

Biography:

Hongmei Luo is the Associate Dean of Research in the College of Engineering and Luke Barry Shires Endowed Professor in Chemical Engineering at New Mexico State University. She received her Ph.D. degree in Chemical Engineering from Tulane University in 2006. Before she joined NMSU in 2009, she was a postdoctoral research associate in Los Alamos National Laboratory. She has authored and co-authored 190 peer reviewed journal publications. Dr. Luo received numerous awards at NMSU, name a few: 2014 Bromilow Award for Teaching Excellence and 2016 Robert L. Westhafer Award for Excellence in Research and Creative Activity.

Electrocatalysts and Electrodes with Atomic Layer Deposition

Shicheng Xu*

Stanford University, USA

Abstract

Polymer-electrolyte-membrane-based hydrogen fuel cell is a promising technology for sustainable powertrains of the future. Cathode, where the electrocatalytic oxygen reduction reaction occurs, poses a significant performance limitation to the device performance. Improving electrical current density under the constraints of catalyst mass loading and electric potential involves highly active catalysts integrated wisely into the electrode structure.

The talk will introduce a workflow of electrocatalysts design, fabrication, and integration with atomic layer deposition. Electrocatalysts designed based on the calculations on the atomic level and reaction pathways can be prototyped with this atomic level additive manufacturing technique. Significant performance benefits are seen. This workflow also allows a greater engineering space for streamlined testing of various catalysts, catalyst support, ionomer, and their combinations. These effects will be discussed.

Biography:

Shicheng Xu is a research scientist in the Nanoscale Prototyping Laboratory at Stanford University. After obtaining his doctoral degree in Mechanical Engineering in 2016, he had since been working on polymer electrolyte membrane fuel cells. His research focuses on electronic structures of catalyst and catalyst systems and transport phenomena in catalyst layer structures. He has ample experience in catalyst fabrication, electrode design, and fuel cell testing (with an accumulated test of 10,000+ hours).

Multinary High Entropy Alloy Nanoparticles from Laser-Based Synthesis as Promising New Class for the Design of Novel Energy Materials.

Sven Reichenberger[1*]
Varatharaja Nallathambi[1,2]
Jacob Johny[1]
Shun-Xing Liang[1]
Stephan Barcikowski[1]

[1] Technical Chemistry I and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitaetsstrasse 7, 45141 Essen, Germany

[2] Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf

Abstract

The laser-based synthesis of colloidal nanoparticles (Fig. 1) is an established, scalable method to design and study the catalytic activity of metal, oxide, and alloy nanoparticles in terms of their pre-adjusted functional nanoparticle properties (size, morphology, oxidation state). [1–3] As a rather novel material class, laser-generated high entropy alloy (HEAs) nanoparticles consisting of more than 5 elements (e.g. FeMnNiCrCo or FeMnNiCrCoMo) have successfully been applied as noble metal-free energy materials in catalysis. [5,6] Hereby, the pulsed laser ablation in ethanol yielded ~8 nm-sized, crystalline high entropy alloy nanoparticles that showed good catalytic activity in the alkaline oxygen evolution reaction (OER). [5] In the present study, acetonitrile was used to further suppress surface oxidationwhile an increasing atom percentage (6-30 at%) of Mo was added to the MnFeCoNiCr system to study the effect of Mo on the electrocatalytic OER and ORR activity.[6] The yielded alloy nanoparticles were found to be amorphous (XRD) which is linked to a significant carbon doping (HR-TEM-EDX) that had previously been discussed to stabilize amorphous nanoparticles during laser-based synthesis[3] . XPS showed a gradual surface enrichment with Mn and a depletion with Mo. The catalytic investigation delivered pronounced activity trends with the composition[7] . Overall, the presented study solidifies the feasibility of the scalable laser-based catalyst synthesis in developing new catalytic systems for industrial and scientific applications.

Biography:

Reichenberger studied chemical engineering at Hochschule Niederrhein. He received his Ph.D. in 2017 at the University of Duisburg-Essen and specialized in the field of laser-based defect engineering during post-doctoral research. He currently is acting leader of a young researcher group at the Institute of Technical Chemistry of the University-Duisburg Essen where he focuses on the laser-based development of defect- and composition engineered metal, alloy, and oxide catalysts for fuel cells, electrolyzers, and thermal redox catalysis.

Phthalocyanines as Efficient Molecular Materials for Energy

Ángela Sastre-Santos[1*]
Adrián Herrero[1]
Desiré Molina[1]
Jorge Follana-Berná[1]
Javier Ortiz[1]

[1]Área de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Elche 03202 (Alicante), Spain.

Abstract

Recently, significant progresses have been achieved in the fabrication of highly efficient perovskite solar cells, while major challenges, such as commercial viablity of exotic materials and their instability, remain as an obstacle. Hole transporting materials (HTMs) represent a tricky choice for the fabrication of efficient solar cells and the cost uneffective Spiro-OMeTAD continue to be so far from the most obvious candidate. Semiconductors molecules, such as metallophthalocyanines (MPcs) [1] appeared as a promising class of p-type material, since they are less expensive and more stable.

In this communication, we will present the synthesis of novel ZnPcs, ZnPc dimers and CuPcs (as efficient, stable, and low cost HTMs in PSCs. [2] The MPcs are substituted with functional groups that possesses a very good solubility in a wide range of organic solvents, adequate HOMO LUMO levels and thus can be applied from solution processing in a wide range of perovskite solar cell devices.

Biography:

Ángela Sastre-Santos is currently Full Professor of Organic Chemistry and Head of the Instituto de Biongeniería at the Universidad Miguel Hernández de Elche. Her research interest focuses on the synthesis of molecular and supramolecular electroactive systems with nano- and biotechnological applications. She is member of the American Chemical Society, Electrochemical Society, Society of Porphyrins and Phthalocyanines, the Spanish Royal Chemical Society and the Spanish Royal Physical Society; within the two latter, she was the President of the Nanoscience and Molecular Material Division (March 2013-May 2021). She has published more than 150 peer-reviewed articles. Awarded by the José Barluenga 2018 Medal of the Specialized Group of Organic Chemistry of the Royal Spanish Society of Chemistry, in recognition of a projection of quality and excellence in her independent research career in Organic Chemistry. Co-founder of the spin-off Anfechem S.L.

Strain-rate-dependent Mechanical Behavior and Energy Dissipation in 3D Printed Liquid Crystal Elastomers

Bo Song[1*]
Kevin Long[1]
Brett Sanborn[1]
Christopher Chung[2]
Kai Yu[2]
Christopher Yakacki[2]

[1]Sandia National Laboratories, USA

[2]University of Colorado at Denver, USA

Abstract

Liquid crystal elastomers (LCEs) are a unique class of polymer with potential for superior energy absorption and dissipation capacities due to solid-state phase transition during deformation, making them as candidate damping materials in applications from vibration to impact. Understanding the energy dissipation characteristic depends on the mechanical stress-strain response under both loading and unloading. Quasi-static loading and unloading stress-strain response can be obtained with a standard material test frame. However, dynamic tests, usually performed with a split Hopkinson pressure bar, provide loading response only for soft polymers. Lack of dynamic unloading response prevents easy determination of the energy dissipation characteristics. In this study, we developed an analytical method for connecting the unloading response to the stress-relaxation behavior such that the unloading stress-strain response and energy dissipation at high strain rates are revealed for the soft polymer. A bench-top test capability was also developed for mechanical characterization at intermediate strain rates. Combining the various test and analytical capabilities, compressive stress-strain responses under both loading and unloading conditions for 3D printed LCEs with monodomain and polydomain, respectively, were obtained. Strain-rate effect on the mechanical behavior and energy dissipation was determined.

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Biography:

Bo Song is currently a Distinguished Member of Technical Staff at Sandia National Laboratories. Bo Song obtained his Ph.D. in Solid Mechanics from University of Science and Technology of China in 2000. Dr. Song's research interests include experimental impact mechanics, mechanics of materials, and dynamic behavior of materials and structures. He has published 2 books and numerous peer-reviewed journal articles. He is currently an Associate Editor of "Mechanics of Materials" journal. Dr. Song has been elected as a Fellow of American Society of Mechanical Engineers (ASME) and International Association of Advanced Materials. (IAAM).

Advances in Materials for Highly Stable and Efficient Composites-Based Perovskite Perovskite Solar Cells

Yoon-Bong Hahn*

School of Semiconductor and Chemical Engineering, Jeonbuk National University, 567 Baekje-daero, Deokjin-gu, Jeonju 561-756, Republic of Korea Email: ybhahan@jbnu.ac.kr (+82-10-7408-8285)

Abstract

For practical use of perovskite solar cells (PSCs) the instability issues of devices, attributed to degradation of perovskite molecules by moisture, ions migration, and thermal- and light-instability, have to be solved. To solve such issues, we developed simple methods for production of functional nanocomposites such as Ag-graphene, perovskite/Ag-graphene, NiO-carbon-graphite, Al2O3/graphene, perovskite-NiO, etc and utilized them for the fabrication of highly stable and efficient PSCs. We reported highly efficient and stable PSCs based on perovskite/Ag-reduced graphene oxide (Ag-rGO) and mesoporous Al2O3/graphene (mp-AG) composites. Compared to a reference cell, the composites-based devices showed an efficiency over 20 %. More importantly, the composites-based champion device without encapsulation exhibited not only remarkable thermal- and photo-stability but also long-term stability with retaining 97-99 % of the initial values of photovoltaic parameters with sustaining ~ 93% of initial PCE over 300 days under ambient conditions. However, most PSCs contain harmful lead (Pb).

Biography:

Hahn is Regents Professor of the Jeonbuk National University (JBNU), Fellows of the Korea Academy of Science and Technology (KAST), the American Ceramic Society (ACerS) and the International Association of Advanced Materials (IAAM). He joined JBNU in 1991, prior to which he worked for LG Metals Research Center for 1988-1991 after he received his Ph.D. in Metallurgical Engineering from University of Utah in 1988. His research interest is synthesis of metal oxide nanostructures and their applications for solar cells, biological sensors, and printed electronics. He holds 17 patents, published over 320 SCI papers (over 14200 citations, h-index over 62), and authored/edited 7 books. He received MCARE Best Research Award 2019 and Woo SeongIl Materials Award 2018 by KIChE, Asian Energy Technology Award 2017 by International Association of Advanced Materials, Rudolf A. Marcus Award for outstanding research in the area of chemical science in 2016, the American Ceramic Society Global Ambassador Award 2016, the Scientist of the Month Award in 2011 by Korea Ministry of Education, Science and Technology, the CBNU's Best Research Professor Award consecutively in 2008-2010, and Top 100 Scientists Award four times in 2005, 2011, 2014 and 2015 accredited by International Biographical Center, Cambridge, UK.

2D-Graphitic like Carbon Nitride Nano Sheets for the Effective Separation of Oil from Water and Wastewater

Rengaraj Selvaraja*
Nada Al Kindia
Faisal Al Marzouqib
Majeda Khraishehc

[a]Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, Oman
[b]Department of Engineering, International Maritime College Oman, Suhar, Oman.
[c]Department of Chemical Engineering, College of Engineering, Qatar University, Doha, Qatar.

Abstract

The separation of oil from water and wastewater, which includes immiscible oil/water and emulsified oil/water mixtures, is a worldwide challenge because of the large amount of oily wastewater produced in many industrial processes and daily life. For the separation of oil and water, filtration technique is considered the most efficient method because of its high separation efficiency and relatively simple operational process. One of the most common methods used for the treatment of oily contaminated water is the filtration method by modified surfaces. In our laboratory, we have developed g-C3N4 via thermal condensation method. These materials were characterized using various advanced chemical and structural techniques including XRD, XPS, UV-DRS, FTIR, SEM, and EDX. In order to separate oil from water, stainless-steel meshes were modified and coated with the prepared g-C3N4 Nano sheets to be used for the separation of oil and water mixture. The nanomaterials coated mesh were functionalized with hydrophobic agents. Different tests were performed to investigate the nature of the coated meshes and their stability and efficiency. After many separation tests, it was found that the most efficient coating among all the modified meshes was g-C3N4, which was functionalized using HDTMS. The separation efficiency of this coated mesh reached nearly 75% and it resulted to fast separation, which happened in a few seconds. In addition, the modified mesh can be used for many cycles and still gives good separation efficiency. These results suggest that the nanostructured coated meshes will be the promising method for the oil spill problem and it will help to remove the oil from the oily contaminated water.

Biography:

RENGARAJ Selvaraj., Ph.D., FRSC, is an Associate Professor of Chemistry in the Sultan Qaboos University, Muscat, Oman with responsibility for teaching, research and consultancy in the field of Analytical and Applied Environmental Chemistry. Dr. Rengaraj graduated from Anna University, Madras, India with a PhD in Chemistry in 1999. He has 30 years of research experience in Materials, Environmental Science and Engineering, particularly in the area of Environmental Nanotechnology, wastewater treatment, water quality analysis, and solid waste management. He has published more than 90 research articles in reputed National, International Journals, and Proceedings (h-index 31) and has been serving as an editorial board member of two International Journals.

Stability and Magnetic Properties of Mn3 Adsorbed on Noble Metal Surfaces: A First-Principles Study.

J. L. Morán-López*[1,2]
E. E. Hernández-Vázquez[1]
S. López-Moreno[1,2]

[1]Science and Engineering Group, National Supercomputing Center, Institute for Scientific and Technological Research, San Luis Potosi, México;

[2]Advanced Materials Division, Institute for Scientific and Technological Research, San Luis Potosi, México

Abstract

The energetics and magnetic properties of Mn trimer adsorbed on the noble metal surfaces Au(111) and Cu(111) is studied by means of first-principles methods within the density functional theory and the generalized gradient approximation. We analyzed the trimer absorbed as a linear chain and forming triangular structures. The triangular trimer can be

adsorbed in two possible configurations on the (111)-fcc surfaces, with different substrate environment, Δ and H. We computed three magnetic configurations, the AF, FM, and non-collinear. The lowest energy configuration, on both metals, is the AF Δ, with an isosceles triangle shape. We analyze in detail the electronic charge spatial distribution and discuss the transfer among the trimer Mn atoms and the surface neighbors. Finally, we computed the energy barriers, along the minimum energy path, that block the transformation from a linear Mn3 arrangement to the Δ configuration on both surfaces.

Biography

José-Luis Morán-López (1950) graduated as a Doctor Rerum Naturalium from the Free University of Berlin in 1977. He is a Full Researcher at the Department of the Advanced Materials Division of the Potosí Institute of Scientific and technological Research. In 1984, he received the John Simon Guggenheim research grant. In 1988, the Organization of American States, bestowed the Manuel Noriega Morales Award in Exact Sciences on him. In 1990, he received the C.V. Raman International Award from the International Centre for Theoretical Physics. In 1992, he won the Alexander von Humboldt Research Fellowship in Germany. In 1996, the Mexican government granted him the National Sciences and Arts Prize.

Characteristics and Packaging of Structural Battery with Carbon Fabric Current Collector

Chun-Gon Kim[1]
Jaechan Pyo[2]
Hyun-Wook Park[1]
Jooseung Choi[1]
Jung-Eon Noh[1]

[1] KAIST, Korea
[2] Georgia Tech, USA

Abstract

Electric vehicles of light weight can be greatly favored by the use of structural battery through efficient use of the internal space as well as weight reduction. We designed and manufactured Li-ion structural battery which is composed of carbon fabric current collectors, cathode and anode active materials, glass fabric separator, liquid electrolyte, and proper packaging materials. The current collector and separator fabrics have dual function of direct load bearing and battery substance. The operation of Li-ion battery structural battery is only possible by realization of proper environment free from humidity and oxygen for the battery compartment sub region inside the composite laminate. The advanced concept lead to the bipolar structural battery. The mechanical as well as electrochemical characterization was carried out for the single cell and bipolar structural battery under tension and bending load. To overcome the limited capability of the structural battery with liquid electrolyte under bending load, some closed cross-sectioned shape like tubular laminated structural battery was fabricated and demonstrated the load bearing and electric energy storage capability.

Biography:

Chun-Gon Kim is currently affiliated to the Department of Aerospace Engineering, KAIST. Following completion of his Ph. D. at KAIST, He served as a senior research engineer in the Composites Laboratory in KIMM (Korea Institute of Machinery and Materials) for 4 years. After joining KAIST faculty in Sept. 1991, He devoted himself to teaching and the research of developing composites for light structure with integrated multi-functions like health monitoring, electromagnetic energy absorbing, electrochemical energy storage, under extreme environment.

Carbon Nanotube Network Formation and its Effect on Rheological and Mechanical Properties of Polymer-Based Nanocomposites

Alen Oseli
Mohor Mihelčič
Lidija Slemenik Perše*

Laboratory for experimental mechanics, Faculty of Mechanical Engineering, University of Ljubljana, Slovenia

Abstract

Within the presented research, we report on carbon nanotube network formation within polymer matrices and its impact on functionality of such nanocomposites, specifically rheological and mechanical reinforcement. Network formation was experimentally observed through plasma etching coupled with electron microscopy as well as rheological analysis, while its impact on functionality was observed through dynamic mechanical analysis and tensile tests (related to mechanical reinforcement). Results showed that the established network is constructed from SWCNT bundles, which geometrically entangle at critical volume fraction Φ_(v,crit). Below Φ_(v,crit), bundles behave as individual units and may align in flow direction. Above Φ_(v,crit), rotation of bundles is constrained by neighboring units, leading to random network configuration that profoundly changes behavior of such nanocomposites, i.e. improving mechanical reinforcement for 1 decade (10x related to modulus).

Biography:

Lidija Slemenik Perše has been fully employed at the Faculty of Mechanical Engineering as a teacher, Head of Chair of Mechanics of polymers and composites and Head of Laboratory for experimental mechanics. She obtained her education at the Faculty of Chemistry and Chemical Technology, University of Ljubljana. Since the graduation her research has been devoted to the field of rheology and mechanical properties of various materials (sol-gel processes, spectral selective coatings, electrolytes, polymeric materials, rheology of food, pharmaceutical materials ...). Currently she is focused on polymer materials and polymer (nano)composites.

Unconventional Piezoelectricity by Flat Phonon Bands in HfO_2

Jinhyeong Jo
Pawan Kumar
Yungyeom Kim
Jun Hee Lee

Ulsan National Institute of Science and Technology (UNIST), Korea

Abstract

Ferroelectric materials are receiving attention in the electronics industry as candidate materials for ferroelectric random-access memories (FeRAM) or nonvolatile resistance memories. In

particular, HfO2 has been studied a lot recently because it has persistently robust ferroelectricity in thin films in contrast to other conventional ferroelectrics (e.g., perovskite oxides like BaTiO3). However, studies on the electromechanical reaction of HfO2 have not progressed significantly yet. Recently, our group showed that HfO2 can be employed as the highest density memory material due to its unusual flat band phenomenon [1]. In this talk, we will discuss the effect of the flat-bands effects on ferroelectric switching and unconventional piezoelectric effects. First, unlike conventional ferroelectrics which have a large coupling between ferroelectric switching and lattice constants, we discovered a surprising phenomenon that the lattice constant does not change at all during the switching. This is mainly because the ferroelectricity of HfO2 is strongly related to the intrinsic effect of the flat bands. The weak interaction of ferroelectric polarization and mechanical lattice expansion will help to overcome deleterious problems in ferroelectric devices such as fatigue usually caused by repetitive switching. Furthermore, we will talk about the origin of the recently reported negative piezoelectricity [2] through DFT combined with a full phonon Hamiltonian and seek experimental routes to maximize the unconventional piezoelectricity by using doping or epitaxial strain.

Biography:

Jinhyeong Jo received his Bachelor of Chemistry from Ulsan National Institute of Science and Technology (UNIST) in 2018. He has various research experiences through his combined MS/PhD periods at UNIST (2018~). Now he is working on discovery of various materials with combination of density functional theory and model simulation.

Poster Presentations

Synthesis of Nepheline from Different Zeolites Prepared from an Aluminum Waste

Aurora López-Delgado*
Isabel Padilla
Maximina Romero

"Eduardo Torroja" Institute of Construction Science, IETcc-CSIC, Spain

Abstract

Nepheline, (Na,K)AlSiO4, is a feldspatoide mineral with excellent mechanical properties, which is used in many industrial applications, specially those relate to the manufacture of glass and ceramics. Nepheline can be obtained by thermal transformation of materials rich in Na, Al and Si as zeolites. This transformation is a complex process that is affected by several factors among others the zeolite structure, the Si/Al ratio, the water content and the extra framework cations. The different mineralogical, chemical, and structural changes occurred during the transformation of zeolite to nepheline, are principally caused by migration and/or ejection of atoms from the crystal lattice of the zeolite, causing chemical stoichiometry variations as well as expansion or contraction of the material. The objective of this paper was to study the transformation of four zeolites, Ana, NaP1, LTA and, SOD into nepheline by thermal treatment. All the zeolites were prepared through a one-step hydrothermal synthesis method, using an Al-rich waste coming from the aluminum slag milling process as the only Al source. The aluminum waste is considered hazardous because of its high reactivity in the presence of water or environmental humidity. The thermal behavior of the parent zeolites was followed by differential thermal analysis and thermogravimetric (DTA-TG). Selected

temperature values were used for the treatment of the zeolite in a muffle to a fixed time. Then, the samples of nepheline obtained were studied by XRD, FESEM and FTIR and the effect of the Al-waste zeolites on the morphological and microstructural characteristics of the nepheline was determined.

Biography:

Aurora López-Delgado (Ph.D in Chemistry, Scientific Researcher at Eduardo Torroja Institute for Construction Science, IETcc-CSIC) has more than 25 years of experience in the synthesis of added-value materials such as glasses, glass-ceramics, ferrites, aluminas, zeolites, etc., using hazardous waste as raw materials. She has co-authored more than 150 scientific publications, 10 patents, and around one hundred presentations at international conferences. Her current research interest includes processing and technological characterization of industrial and mining wastes in order to develop processes to get added-value materials, and also, in the application of concentrated solar energy to high temperature processes.

Thermoelectric properties of two-dimensional materials observed by tuning energy states

Hyunjung Lee

School of Materials and Engineering, Kookmin University, Seoul, Republic of Korea

Abstract

We observed the carrier transport properties of thermally reduced graphene oxide (TrGO) as a function of reduction temperature. The transfer curve of a field-effect transistor fabricated with TrGO exhibited ambipolar properties, and the charge neutrality point of TrGO was shifted from negative to positive as the reduction temperature increased. Furthermore, as revealed in Arrhenius plots of the carrier densities and carrier mobilities, TrGO behaved as a metallic conductor at all reduction temperatures. To investigate the effect of reduction temperature on the thermoelectric properties of TrGO, the Seebeck coefficients of the fabricated TrGOs were calculated from the transfer curve using Mott's equation for metallic materials. The calculated Seebeck coefficients at zero gate bias were compared with the measured coefficients in TrGO bulk films. Thermoelectric properties of the measured and calculated coefficients showed similar trends with increasing reduction temperature, and the charged carrier transport (i.e., the energy states) of TrGO can be tuned by varying the reduction temperature without doping with impurities. In other study, WS2 particles were hybridized with highly conductive reduced graphene oxide (rGO) particles. The inclusion of rGO provides conductive paths for the transfer of carriers in the composites, and thus, this led to an increase in their electrical conductivity. The hybrid material of WS2/rGO, as a function of the weight percentage of rGO, was fabricated by spark plasma sintering. Moreover, two-dimensional structures of the materials contributed to the induction of phonon scattering and resulted in steady k in spite of enhanced σ with increased rGO content.

Biography:

Hyunjung Lee is a Professor of the School of Materials and Engineering at Kookmin University. She received her PhD degree in 2001 from Pohang University of Science and Technology, majoring in polymer chemistry. After post-doctoral periods in University of Illinois at Urbana-Champaign (UIUC) and Massachusetts Institute of Technology (MIT), Prof. Lee developed a research career at Korea Institute of Science and Technology (KIST) as a principal research scientist. Now she is a full professor at Kookmin University since 2010. Prof. Lee's research area covers chemical sensors and diverse energy devices such as solar cells and thermoelectric devices.

Synthesis and assessment of a new micro-structured fluorescent sol-gel architecture intended for optical sensing

Ibtihel Marzouk[1,2]
David Riassetto[1]
Alain Morand[2]
Davide Bucci[2]
Michel Langlet[1]

[1]Univ. Grenoble Alpes, CNRS, Grenoble INP, LMGP, F-38000 Grenoble, France
[2]Univ. Grenoble Alpes, CNRS, Grenoble INP, IMEP-LAHC, F-38000 Grenoble, France

Abstract

We present a fluorescent wave-guiding micro-structured architecture on glass entirely elaborated by sol-gel processing. This architecture is composed of a channel waveguide doped with an oxygen sensitive fluorophore (Rudpp) and endowed with diffraction gratings. It particularly takes advantage of a high refractive index titanium oxide based sol-gel photoresist that can be imprinted through a single photolithography step. The gratings enable to inject the green excitation signal in the axis of the waveguide core and to extract the red signal emitted by Rudpp toward a photodetector. We firstly present the multi-step elaboration process leading to this architecture. Opto-geometrical properties of the channel waveguide and diffraction gratings are assessed and optimized on the basis of optical and AFM characterizations. According to these properties, best injection and extraction angles of the excitation and emission signals have been determined thanks to optical simulation. Then, we present fluorescence measurements performed in wave-guiding configuration using a specifically designed optical bench. These measurements demonstrate that the waveguide enables efficient propagation of light at the excitation and emission wavelengths of the fluorophore and that the diffraction gratings are compatible with efficient injection and extraction of the excitation and emission signals. This work constitutes a promising first step towards a new class of oxygen sensors based on the wellknown principle of oxygen driven extinction of the Rudpp fluorescence.

Biography:

Technology is my true passion. I believe scientific research is a journey, we are all learning and constantly improving. Working in a team allows me to move forward and go further. My name is Ibtihel Marzouk. I am in my third year of thesis at Institute of Engineering University Grenoble Alpes (Grenoble-INP). My thesis entitled Synthesis and evaluation of a new microstructured fluorescent sol-gel architecture intended for optical detection, takes place at the Laboratory of Physics of Materials and Engineering (LMGP) and at the Institute of Microelectronics Electromagnetism and Photonics - Laboratory of Hyperfrequencies and Characterization (IMEP-LAHC).

Humidity Resistant and Mechanically Enhanced Graphene Oxide (GO)/Poly(ionic liquid) (PIL) Composite Films

Jian Chang[1*]
Miao Zhang[2]
Qiang Zhao[3]
Liangti Qu[4]
Jiayin Yuan[5]

Department of Materials and Environmental Chemistry, Stockholm University, Sweden.

Abstract

Graphene oxide (GO) is a classic two dimensional (2D) building block that can be used to develop high-performance materials for numerous applications, particularly in the energy and environmental fields. Currently, the precise assembly of GO nanosheets into macroscopic nanocomposites of superior strength and toughness is desirable, and faces challenges and trade-offs. Herein, we exploited the freshly established polycationitrile method as a powerful molecular crosslinking strategy to engineer ultratough and ultrastrong GO/polymer composite films, in which a covalent triazine-based network was constructed in a mild condition to reinforce the interface between GO nanosheets. The tensile strength and toughness reached 585 ± 25 MPa and 14.93 ± 1.09 MJ m-3, respectively, which, to the best of our knowledge, are the current world records in all GO-based composite films. As an added merit of the tailor-made polymer crosslinker, the high mechanical performance can be maintained in large part at an extremely high relative humidity of 98%. This emerging interface-engineering approach paves a new avenue to produce integrated strong-and-tough 2D nanocomposite materials that are useful in aerospace, artificial muscle, energy harvesting, tissue engineering and more.

Biography:

Jian Chang is currently a PhD student at Department of Materials and Environmental Chemistry, Stockholm University, Sweden. From 2016 to 2019, he was a research engineer at King Abdullah University of Science and Technology, Saudi Arabia. He received his B.Sc. degree in Applied Chemistry in 2013 and M.S. degree in Polymer Chemistry and Physics in 2016, both from Jilin University, China.

Development of niclosamide-based COVID-19 therapeutic reagent using porous silicon nanoparticle

Jae Seung Kang

Department of Anatomy and Cell Biology, Seoul National University College of Medicine, Seoul, 03080, Korea.

Abstract

Porous Silicon Nanoparticles (PSiNPs) can be used in effective drug delivery system after loading of drugs on its porous structure. In addition, its enhanced permeability and retention (EPR) effect, one of characteristics of nanoparticles, increases the effectiveness of drugs and decreases of cytotoxicity. The recent global emergence of COVID-19 caused by SARS-CoV-2 and its variants has led to an immediate demand for a drug to treat the virus infection. Therefore, drug repositioning is receiving a lot of attention in that it can reduce the time and cost required for develop new drugs. Niclosamide and artesunate are suggested as potential

drugs for COVID-19 treatment, but their cytotoxicity and physical limitations are remained to be solved problem regardless of effectiveness. Therefore, we examined whether PSiNPs could increase of effectiveness and decrease of cytotoxicity of niclosamide and artesunate for COVID-19 treatment. After fabrication of PSiNPs from silicon wafer through electrochemical etching, particle size and shape upon surface modification using with DLS and TEM was examined. As a result, three types of PSiNPs, PSiNPs-H, PSiNPs-COOH, and PSiNPs-NH2, were generated. Among them, PSiNPs-NH2 was selected, since it showed highest absolute value of zeta-potential. Niclosamide was effectively loaded into PSiNPs-NH2, with the loading efficiency of 32.7% ± 2.2, but artesunate was not. The suppressive effect of niclosamide only and niclosamide-loaded PSiNPs-NH2 on the replication of delta variant of SARS-CoV-2 in Vero E6 was investigated by plaque assay. Interestingly, niclosamide-loaded PSiNPs-NH2 more effectively suppressed the replication of delta variant of SARS-CoV-2 without cytotoxicity than niclosamide only. Additionally, I have secured PSiNPs with the conjugation IgG and scFv form of ACE2, a critical receptor during SARS-CoV-2 infection. Therefore, this result suggests that niclosamide loaded PSiNPs and ACE2 antibody conjugated PSiNPs can be used as effective drug delivery platform for niclosamide-based COVID-19 treatment.

The End Day-1

Keynote Presentations

Optical Properties of 2D Semiconducting Materials: Trions, Excitons, Polaritons

Vasili Perebeinos

Electrical Engineering Department, University at Buffalo, State University of New York, 230 Davis Hall, Buffalo, USA

Abstract

Atomically thin two-dimensional transition metal dichalcogenide monolayers are direct bandgap semiconductors with the rich interplay of the valley and spin degrees of freedom. A strong Coulomb interaction leads to tightly bound electron-hole pairs or excitons and two-electrons one-hole quasiparticles or trions. We solve the two-particle and three-particle problems for the wavefunctions for excitons and trions in the basis set of the model Hamiltonian for single particles. The calculated linear absorptions [1], photoluminescence [2] spectra, as a function of doping and temperature, explain the experimental data in 2D monolayers and predict novel spectroscopic features [3] due to the many-body Coulomb interactions. The nonlinear dynamics follows from the solution of the time evolution equations for the density matrix. Excitons qualitatively change the nonlinear dynamics leading, in particular, to a huge enhancement of the second harmonic generation (SHG) signal. The SHG polarization angular diagram and its dependence on the driving strength are predicted to be very sensitive to the type of the exciton state [4].

Biography:

Vasili Perebeinos is a Professor of the Electrical Engineering Department at the University of Buffalo. During his research career, he became a Fellow of the American Physical Society. He received the highly competitive "IBM Research Technical Accomplishment" award three times and the best paper award by the IBM Materials Research Council. Perebeinos's research interests are in theory and simulations of advanced materials and nanostructures for electronics and optoelectronics, specifically novel 2D materials, and 1D carbon nanotubes. He is the author or co-author of over 90 journal articles cited over 15,500 times (h-index 50 – google scholar).

Progress in Water Desalination Using All-Carbon Membranes

David Tománek

Physics and Astronomy Dept., Michigan State University, East Lansing, MI 48824, USA

Abstract:

Whereas water itself is bountiful on Earth, much of it requires treatment to make it suitable for human consumption. Lack of potable water is currently the leading cause of death, ahead of any disease. Recent progress in fabricating nanostructured carbon allotropes may bring a long-awaited paradigm shift in designing membranes that would make efficient desalination

of salt water using reverse osmosis and filtration of contaminated water possible. A previously unexplored membrane design [1] based on a unique layered assembly of carbon nanostructures including graphite oxide (GO), buckypaper consisting of carbon nanotubes, and a strong carbon fabric should provide high mechanical strength and thermal stability, resilience to harsh chemical cleaning agents and electrical conductivity, thus addressing major shortcomings of commercial reverse osmosis membranes. Microscopic insight into the critical permeation of water molecules in-between GO layers and across in-layer vacancy defects in graphitic carbon can be obtained using ab initio density functional theory calculations. Results of these computational studies elucidate the reason for selective rejection of solvated Na+ ions in an optimized layered all-carbon membrane.

Biography:

David Tománek is a U.S.-Swiss physicist of Czech origin and researcher in nanoscience and nanotechnology. He is Emeritus Professor of Physics at Michigan State University. He is known for predicting the structure and electronic properties of surfaces, atomic clusters, nanotubes, nanowires and graphene, and two-dimensional materials including phosphorene. His current focus is water desalination. He initiated a series of Nanotube (NT) conferences and a Gordon Research Conference on Two-dimensional electronics beyond graphene. He is a Fellow of the American Physical Society, recipient of the Alexander-von-Humboldt Senior Scientist Award in Germany and the Carbon Award for Life-Time Achievement in Japan.

Oral Presentations

Flexible and Wearable Sensors based on Soft Conductive Materials for Human Motion Monitoring

Zhengtao Zhu*
Obiora Onyilagha

Department of Chemistry, Biology, and Health Sciences, South Dakota School of Mines and Technology, USA

Abstract

Wearable systems consisted of conformable and lightweight biomedical/strain sensors, power sources, and wireless modules have broad application potentials in human motion monitoring, medical, human-machine interface, safety, and soft-robotics. Our research in this area focuses on combination of conductive nanofibers/polymers and soft scaffold materials (such as elastomers and hydrogels) to design multi-component and multi-functional composite materials. In this talk, I present our recent work on electrospun nanofibers as a key component in flexible and wearable electronic devices. Using electrospun carbon nanofiber as a piezoresistive element, we have demonstrated highly stretchable strain sensors by embedding freestanding electrospun carbon nanofibrous mat in an elastomer for human motion monitoring. The morphology, mechanic property, and sensor responses of the stretchable sensors were investigated. Highly compressible tactile sensor for electronic skin application is demonstrated using three-dimensional (3D) conductive sponge prepared by freeze-drying of the building blocks of shortened electrospun nanofibers. The sponge composed of these electrospun nanofibers is ultralight with hierarchical pores; under compressive strain, the resistance change of the 3D conductive sponge shows high sensitivity and stability over a wide range of compressive strain. Sensors fabricated using these soft

conductive materials are attached to the different parts of human body; the capabilities of these devices to detect human motions including speaking, finger bending, elbow bending, and walking are evaluated. Furthermore, prototype tactile sensory array based on these pressure sensors is demonstrated.

Biography:

Zhengtao Zhu is an Associate Professor of Chemistry and Head of the Department of Chemistry, Biology, and Health Sciences at South Dakota Mines. Dr. Zhu earned his Ph.D. in Materials Chemistry from the State University of New York in 2002. He was a postdoctoral research scientist at the University of Illinois at Urbana-Champaign and Cornell University before he joined South Dakota Mines in 2006. Dr. Zhu's research focuses on nanomaterials and conducting polymers, chemical/biological sensors, flexible electronics, energy storage materials, and advanced manufacture/nanofabrication. Dr. Zhu has more than 80 publications in a variety of research areas and his research has been funded by NSF, NASA, ACS, EPA, and private companies.

Novel pectin-based hydrogel systems for biomedical applications

Wujie Zhang

Milwaukee School of Engineering, Milwaukee WI 53202

Abstract

Pectin is a naturally occurring polymer composed of galacturonic acid with carboxyl groups, mostly from citrus fruit and apple peels. Due to its excellent biocompatibility and easily modifiable, pectin-based hydrogel systems show great promise in various biomedical applications. Pectin-based temperature-responsive bioink has been developed without using UV-light or other resources. Moreover, microsphere-incorporated pectin-based bioink can be used for vascularized tissue engineering. A Pectin-based microsphere system has been designed for colonic drug delivery due to its enzymatic responsiveness. Administered orally, the microsphere system can bypass the stomach and small intestine and release the encapsulated bioactive molecules through the microsphere degradation by the colonic microorganisms. Lastly, pectin-oligochitosan microspheres exhibit a red-blood-cell shape and have been developed for novel oxygen therapeutics design-mimicking natural red blood cells. The hemoglobin encapsulation efficiency has been determined to be over 99% and high retention (< 2% within 48 hr).

Biography:

Wujie Zhang is an associate professor of Biomolecular Engineering at the Milwaukee School of Engineering (MSOE). His scholarly work and research span biomaterials, micro/nanotechnology, cellular and tissue engineering, drug delivery, and cancer treatment. As PI, Dr. Zhang was awarded a national NSF I-Corps grant relating to the commercialization of an artificial-red-blood-cell product. Dr. Zhang was recognized by the ASEE's Prism magazine as one of 20 high-achieving researchers and educators under 40 (2018) and the Milwaukee Business Journal 40 under 40 (2019).

Biocementation of Soils: from Laboratory Tests Towards Field Application

Rafaela Cardoso

Instituto Superior Técnico, University of Lisbon, Portugal

Abstract

Biocementation, or Microbially Induced Calcite Precipitation, MICP, consists in using non-pathogenic bacteria to produce calcium carbonate (biocement). This biocement clogs the soil pores and bonds its grains, and for this reason the soil properties change with the treatment. Several are the applications of the treatment, such as soil strengthening and soil improvement for foundations, prevention of internal erosion in earth dams, and resistance to erosion. The main experience on this technique is being earned in laboratorial tests, where bacteria species and dosages to use are optimized and treatment protocols are defined, but there are already some large scale and field tests showing the viability of this technique, which is being already explored by some companies. Laboratorial tests continue to be fundamental for the field application of this technique, to study durability, improve the efficiency of the treatment, define quality control protocols and provide data to calibrate design tools. The use of experimental tests to provide data directly related with field application is explored in this presentation, after a brief introduction to biocementation, challenges, advantages and limitations.

Biography:

PhD in Civil Engineering, Associate Professor with Habilitation at Instituto Superior Técnico (IST), Lisbon University, Portugal. Has 26 papers in international ISI/Scopus journals, 4 book chapters in international publications and more than 50 international conference papers (Scopus h_index=13). Invited for 16 lectures (4 national and 12 international). PI of 3 National Research Projects (2 ongoing) and member of several national research projects. Participation in several consultancy projects for companies. Main research interests are unsaturated Soils and soil-atmosphere interaction, structured soils, artificially cemented soils, biocementation, coupled hydro-mechanical, electro-hydro-mechanical and chemo-hydro-mechanical behaviour of clayey soils.

The Fast Hypoosmotic Permeability Response by 'Smart' Bacterial Envelopes

Sergei Sukharev*

University of Maryland, College Park, USA

Abstract

Bacteria survive exposure to drastically hypoosmotic media, such as rain water, by quickly releasing small metabolites and thereby reducing the hydrostatic pressure inside the cell. The release system comprises two major tension-activated channels, MscS and MscL, residing in the cytoplasmic membrane. The 3-nm MscL activates at near-lytic (10-15 mN/m) tensions, whereas the smaller (1.6-nm) MscS opens at moderate tensions (~7 mN/m) and closes last to terminate the immense response characterized by a >108 fold permeability increase. We start the overview by considering the completely dehydrated states of the closed pores that allow these channels to stay leakproof under resting conditions in cells normally hyperpolarized to -200 mV. We will consider the energetic and spatial scales for activation and positions of activation barriers defining the kinetics of release. The selectivity mechanisms will be

described in conjunction with the repertoire of permeable intracellular osmolytes. The last part will emphasize the critical capacity of MscS to proceed from the closed to the inactivated state, which is non-conductive and tension-insensitive. Inactivation occurs under moderate tension near the MscS activation threshold and is sharply augmented by both increased macromolecular crowding pressure in the cytoplasm and by depolarizing voltages. Dissection of the dynamics of the entire MscS-MscL channel population using patch-clamp shows that during the release phase, MscS plays an important role of reducing membrane tension below the MscL threshold, thus silencing the large channel. When MscS reaches its own threshold, it enters the silent inactivated state, driven by three separate inputs enabling the self-shutting-off capacity.

Biography:

Sergei Sukharev received his Doctorate in Biophysics from Moscow State University. He started as a postdoctoral fellow at the Frumkin Institute of Electrochemistry (Moscow). In 1991 he moved to the US and continued his training in membrane biochemistry at the University of Wisconsin-Madison. During that period, he isolated and cloned the first tension-activated channel MscL. In 1997 he joined the faculty of the Biology Department at the University of Maryland where he teaches and maintains his dynamic research on bacterial osmoadaptation, mechanical responses mediated by membrane proteins, and effects of lateral pressure on membrane partitioning and permeation of drugs.

II-VI Based Organic-Inorganic Hybrids: Structures, Properties, and Stability

Yong Zhang

The University of North Carolina at Charlotte, USA

Abstract

A group of organic-inorganic hybrid nanostructures [1], for instance, β-ZnTe(ML)0.5, where ML = CnN2H2n+4 (n = 0, 2-4), have been shown to exhibit practically perfect structural ordering, manifesting as high crystallinity comparable to that of a typical high quality III-V or II-VI binary. For instance, β-ZnTe(C2N2H8)0.5 has been shown to have a 20-30” XRD rocking-curve linewidth, below 1 cm-1 low-temperature Raman linewidth, and free below-bandgap PL emission [2]. More interestingly, it offers various highly desirable properties, e.g., room temperature excitonic emission due to a large exciton binding energy estimated to be over 200 meV, strongly enhanced optical absorption as high as 106 cm-1 [3], close to 100% internal quantum efficiency in room-temperature photoluminescence [2], broad temperature range zero-thermal expansion [4], and much reduced density and dielectric constants [3]. These novel properties suggest many potential applications, including room-temperature exciton-polariton condensation, optical switching, efficient UV emission, detection, and sensing, transparent p-type conductive material. It uniquely exhibits high stability among the hybrids with a shelf life over 15 years and practically infinitely long intrinsic life [2]! [1] X.Y. Huang et al., J. Am. Chem. Soc. 125, 7049 (2003). [2] T. Ye et al., ACS Nano 15, 10565 (2021). [3] Y. Zhang et al., Phys. Rev. Lett. 96, 026405 (2006). [4] Y. Zhang et al., Phys. Rev. Lett. 99 215901 (2007).

Biography:

Yong Zhang is Bissell Distinguished Professor in Electrical and Computer Engineering Department, UNC-Charlotte. He received his B.S. and M.S. degrees from Xiamen University and Ph.D. from Dartmouth College, all in Physics. He did his postdoc at NREL and was a Senior Scientist before he took the current position. His research interests include electronic and optical properties of semiconductors and related nanostructures, organic-inorganic hybrid materials, impurity and defects in semiconductors, and novel materials and device architectures for applications in optoelectronics, energy, and electronic-photonic integrated circuits. He has published more than 240 papers and book chapters. He is an APS Fellow.

Electrical Field-Applied to Nanotubular TiO2-Layers for Guided Tissue Engineering

Jung Park[1*]
Anca Mazare[2]
Patrik Schmuki[2]

[1]Div. of Molecular Pediatrics, Children's hospital, Erlangen-Nuremberg University, Germany;
[2]Department of Materials Science, WW4-LKO, Erlangen-Nuremberg University, Germany.

Abstract

In regenerative medicine, in spite of the long history over 50 years and beneficial effects of electric fields on bone regeneration, the electric stimuli-sensing mechanism in bone was poorly understood. Biocompatible TiO2 implant surfaces can be the potential candidate of substrate for electric field-guided bone regeneration, since TiO2 implant has been widely used in dental and orthopedic fields. Previously, we have developed vertically aligned TiO2 nanotube layers where individual tube diameters were precisely adjustable in the range of 15–150 nm using anodic self-ordering oxidation of titanium at different voltages. Further, we demonstrated that osteogenic differentiation of mesenchymal stem cells is stimulated responding to the topographic cues from ordered TiO2 nanotube layers with distinct nanoscale geometry. We will introduce our recent study to investigate the combination of an electric field with a nanoscale topographic cue of TiO2 nanotube surfaces, and their delivery system to induce synergistic osteogenic stimulation for guided bone tissue engineering.

Biography:

Group leader, Div. of Molecular Pediatrics, Children's hospital, University of Erlangen-Nuremberg, Germany his Main research fields: Molecular biology, stem cells, stem cell microenvironment, bone tissue engineering, autologous stem cell transplantation, biomolecule-coated implant, stem cell behavior at nanoscale

Magnetoplasmonic Au-Fe3O4 Nanoheterodimers for X-ray Triggered Cancer Therapy

Stefanie Klein[1*]

[1]University Erlangen-Nuremberg, Germany

Abstract

Radiosensitizers increase the susceptibility of tumors to radiation-induced injury. High atomic number nanomaterials such as gold nanoparticles enhance the effectiveness of conventional radiation therapy due to their high X-ray absorption coefficient. The interactions of X-rays with drug-loaded superparamagnetic Fe3O4 nanoparticles causes the release of drugs into the cytosol. Simultaneously, X-radiation activates the catalytic activity of the Fe3O4 surfaces. Surface standing Fe2+ and Fe3+ ions effectively catalyze the Fenton and Haber-Weiss reaction.

Due to alterations in the reactive oxygen detoxifying enzyme levels, cancer cells often have elevated H_2O_2 levels. H_2O_2 is converted to the highly toxic OH• radical, so that the Fe^{2+} driven Fenton reaction is favored. However, under ambient conditions surface Fe^{2+} ions gradually oxidize to Fe^{3+} ions. Fe_3O_4 nanoparticles epitaxially grown on gold nanoparticles yielding Au-Fe_3O_4 nanoheterodimers exhibit enhanced Fenton catalytic activity. In addition, X-rays release electrons from the gold component, leading to synergistic formation of reactive oxygen species.

Since the as-synthesized nanoheterodimers are surface stabilized with oleic acid/oleylamine, ligand exchange is required for water solubility. The ligand exchange with nitrosyl tetrafluoroborate yields NO^+-functionalized nanoheterodimers, which provide synergistic generation of reactive oxygen and nitrogen species under X-ray exposure. To obtain nanoheterodimers with a radioprotective function in healthy cells, the nanoheterodimers are functionalized with the natural antioxidant and anti-cancer drug caffeic acid. Caffeic acid-functionalized nanoheterodimers are shown to act as radioprotectors in healthy breast epithelial cells, but as X-ray dose enhancers in breast cancer cells in (2D) monolayer cell cultures as well as in (3D) multicellular spheroids.

Biography:

Stefanie Klein actually works as a senior scientist at the Department of Chemistry and Pharmacy, Physical Chemistry I, University Erlangen-Nuremberg. During her PhD thesis, she optimized the application of silicon quantum dots as a transfecting agent for ABCB1-siRNA. During her post-doctoral research in La Plata, Argentina and Lubljana, Slovenia amine-terminated ultra-small and iron doped silicon nanoparticles for radiation therapy were developed. Her current research focused on ferrite and noble metal iron oxide nanoparticles to be used as synergistically X-ray dose enhancers and drug carriers in multimodal cancer therapy.

Developing Ir(III) Complexes as Photosensitizers for Photodynamic Therapy

Wenfang Sun

North Dakota State University, Fargo, ND

Abstract Not Available...!

Antibacterial activity of bacteriophages-loaded hydrogels: on the importance of mechanical stiffness

Grégory Francius[1*]
Manon Cervulle[1]
Eloïse Clément[1]
Xavier Bellanger[1]
Christophe Gantzer[1]
Jérôme F.L. Duval[2]

[1]Université de Lorraine, CNRS, LCPME, F-54000 Nancy, France
[2]Université de Lorraine, CNRS, LIEC, F-54000 Nancy, France.

Abstract

The elaboration of novel and efficient hydrogel-based materials with antimicrobial properties requires a refined control of their defining physicochemical features, which includes mechanical stiffness, so as to properly mediate their antibacterial activity. In this work, we

design hydrogels consisting of polyelectrolyte multilayer films for the loading of T4 and φX174 bacteria-killing viruses, also called bacteriophages. We investigate the anti-adhesion and bactericidal performances of this biomaterial against Escherichia coli, with a specific focus on the effects of chemical cross-linking of the hydrogel matrix which, in turn, mediates the hydrogel stiffness. Depending on the latter and on phage replication features, it is found that the hydrogels loaded with the bacteria-killing viruses make it possible both contact-killing (targeted bacteria are those adhered at the hydrogel surface) and release killing (planktonic bacteria are the targets) with ca. 20% to 80% efficiency after only 4 hours incubation at 25°C, as compared to cases where hydrogels are free of viruses. We further demonstrate the lack of dependence of virus diffusion within the hydrogel and of the maximal viral storage capacity on the hydrogel mechanical properties. In addition to the evidenced bacteriolytic activity of the phages loaded in the hydrogels, the antimicrobial property of the phages-loaded materials is shown to be partly controlled by the chemistry of the hydrogel skeleton and, more specifically, by the mobility of the peripheral free polycationic components, known for their ability to weaken and permeabilize membranes of bacteria, the latter then becoming 'easier' targets for the viruses.

Biography:

Grégory Francius is a CNRS research director at the LCPME laboratory (UMR 7564) of the University of Lorraine, and is expert on combined microscopy and spectroscopies techniques applied to biomaterials. His research is at the interfaces of different disciplines ranging from physical-chemistry of materials to the nanoscale investigation of biophysical and biochemical phenomena involved at biological interfaces. More particularly, he designed new smart antimicrobial materials for biomedical field applications. He has published more than 100 peer-reviewed journal papers and edited 3 books.

Fatigue analysis of shape memory alloys

Ziad MOUMNI*

UME-ENSTA-Paris, Institut Polytechnique de Paris, 828 boulevard des Maréchaux 91120, Palaiseau France

Abstract

Shape memory alloys (SMAs) exhibit interesting properties when subjected to mechanical or thermal loadings. For instance, they can accommodate large recoverable strains, or recover their shape by simple heating after being inelastically strained. In many applications (aerospace, aeronautic, energy, automotive, biomedical) shape memory alloys are subjected to cyclic loadings, which could induce failure of the SMA structure by fatigue. Hence, a better understanding of fatigue of SMAs thus seems important in order to further promote the use of these materials in high-tech applications.

In this talk, we present a comprehensive approach for fatigue of SMAs developed in our research group the last 10 years. It includes four steps: i) the development of an accurate constitutive model to predict the stabilized thermo-mechanical state of a SMA structure under cyclic loading; ii) an energy-based criterion to predict low-cycle fatigue of SMAs, iii) a shakedown-based fatigue model to predict high-cycle fatigue of SMAs and iv) a structural optimisation procedure to design SMAs components with respect of fatigue. Our approach takes into account the main features related to the unusual SMAs behaviour such as the

strong thermo-mechanical coupling resulting from the dependence of the fatigue lifetime on the loading frequency.

Biography

Ziad MOUMNI is Professor of mechanical engineering at ENSTA-Paris. His research fields deal with the theoretical and numerical modeling of the behavior, fatigue and fracture of non-linear materials and structures presenting multi-physics and thermo- mechanical coupling, namely smart materials and structures. In 2012, he created the research group DOSMS (Design of Smart Materials and Structures) which is today internationally recognized for its activities in the field of smart materials and structures. He is involved in many industrial applications in the field of transportation (automotive, aeronautics and space) and energy. He published more than 100 papers in international journals.

Shallow Thin Film Encapsulation with Stoichiometric Silicon Nitride and ORMOCER Double Layers, with Applications to Foldable and Stretchable OLED

MunPyo Hong[1,2*]
Jaewan Park[1]
SeungMin Shin[1]
Gerhard Domann[3]
Daniela Collin[3]

[1]Department of Applied Physics, Korea University, Korea
[2]Advanced Material Transfer Evaluation Center, Korea
[3]Fraunhofer Institut für Silicatforschung, Germany

Abstract

We present the simplest structure of thin film encapsulation (TFE) composed by double layers (or one dyad) with the stoichiometric silicon nitride (S-SiNx) and the inorganic-organic hybrid polymer (named as ORMOCER) thin films for the foldable & stretchable OLED.

This study reveals that the stoichiometricity of SiNx-TFs significantly governs the packing density and water vapor transmission rate (WVTR), and it can be controlled by chemical reactions accompanied by the removal of oxygen impurities with a nitrogen neutral beam (N-NB). Here, oxygen contents of SiNx-TFs are reduced through formation of volatile NOx, and their amount is dominated by the energy of the N-NB. The single-layered stoichiometric SiNx-TFs with a thickness of 100 nm provides WVTR of 6.2 × 10–6 g/(m2day), with a density and composition ratio of N/Si stoichiometry at 3.14 g/cm3 and 1.33, respectively. ORMOCER polymers are synthesized by hydrolysis / polycondensation reactions; the inorganic backbone is responsible for excellent dielectric, thermal and chemical stability, while the organic side groups introduced by the selection of precursor influence curing reactions and processing, coating behavior, Young's moduli, and dielectric permittivities. Additionally, the ORMOCER polymer thin films show higher plasma-resistant property during reactive ion etching of the SiNx-TFs with ambient of CF4/O2/Ar. The double-layers TFE with the S-SiNx and the ORMOCER thin films with a thickness of 0.1 & 3 mm, respectively, has an improved WVTR of 2.3 × 10-6 g/(m2day) due to enhancement by cured interface with Si networks in ORMOCER polymer top coating layer.

Biography:

MunPyo Hong received the Ph.D. degree in Engineering Physics (Plasma Physics) from the

University of Wisconsin-Madison in 1995.

He is currently a Professor with the Division of Display and Semiconductor Physics and a Director of Advanced Material Transfer Evaluation Center, Korea University, and has worked in Samsung Electronics LCD R&D Center (currently Samsung Display) as Principal Engineer/ Group Leader/ Project Manager from 1995 to 2006. His research interests focus on the development of high resolution stretchable & wearable display, new plasma process, organic electronic device & gas barrier coating, next generation TFTs and e-skin technology including e-papers

Plasma Nitriding of Additive Manufactured Metallic Materials to Improve the Corrosion and Wear Resistance

Matjaž Godec[1*]
Bojan Podgornik[1]
Francisco Ruiz-Zepeda[2]
Aleksandra Kocijan[1]
Črtomir Donik[1]
Danijela Skobir Balantič[1]

[1] Institute of Metals and Technology, Slovenia
[2] National Institute of Chemistry, Slovenia

Abstract

Many different steels, including tool steels, can be produced using additive-manufacturing processes. Steels made with selective laser melting (SLM) in some cases have mechanical properties even better than those made conventionally. The reason for the improved mechanical properties lies in the texture, nano-oxides and in the unique microstructure due to the rapid solidification that results in the formation of a dislocated cell structure. For most tool steels, as well as other steels, the corrosion and wear properties are very important. That is why various surface-hardening procedures are increasingly used. Plasma nitriding greatly improves the corrosion as well as the wear properties. Because steels made with SLM have a unique microstructure; however, processes such as plasma nitriding may behave differently in the case of additive-manufactured materials. We will present research on the plasma nitriding of various tool steels (MS1, H11 and H13) as well as other steels such as stainless steels and Inconel. The microstructural results of the compound and diffusion layer will be presented and compared with conventional material. In addition, we will also consider the influence of different heat treatments on the development of the nitride layers. The results will be supported by corrosion and wear measurements.

Biography:

Matjaž Godec has completed his Ph.D at University of Ljubljana, Slovenia, at Faculty of Natural Science and Engineering, Metallurgy in 1997. Since 2011 he has been a director of Institute of Metals and Technology in Ljubljana Slovenia. He has published more than 130 original scientific papers in reputed journals and more than 300 reports and expertise for industrial partners. He had 6 international projects and 8 national projects. His h-index is 19 and he has 1340 citations. He is also first assistant chief editor of the journal Materials Science and Technology and the main organizer of International Conference on Materials and Technology

Hybrid nanoparticles for Spectral photo counting scanner CT From in vivo imaging to therapeutic applications.

Frederic Lerouge[1*]
Frederic Chaput[1]
Szilvia Karpatit[1]
Stephane Parola[1]
Marc Vandamme[2]
Emmanuel Chereul[2]
Pia Akl[3]
Salim Si-Mohamed[3]
Loic Boussel[3]
Philippe Douek[3]

[1]Univ Lyon, Ens de Lyon, CNRS UMR 5182, UCB Lyon 1, Laboratoire de Chimie, France
[2]VOXCAN, 1 Avenue Bourgelat, 69280 Marcy-l'Étoile, France
[3]CREATIS, UMR CNRS 5220, U630 Inserm, Hôpital Neuro-cardiologique, Lyon]

Abstract

Spectral Photon Counting Computed Tomography (SPCCT) is a new imaging modality, currently in development. The SPCCT scanner is an evolution of the conventional CT scanner allowing energy discrimination with high spatial resolution. Its main asset is the ability to map and quantify elements based on their K-edge. For that modality, the use of new types of contrast agents is therefore necessary.

We are focusing our interest on the design and the study of contrast agents suitable for both imaging modalities classical scanner CT and SPCCT. In that context, rare earth fluoride nanoparticles are of particular interest. The presentation will focus on the design of gadolinium-based nanoparticles (GdF3) functionalized with organic ligands. These particles can be used as blood pool imaging agents at preclinical stage. Sensitivity results and biodistribution studies after in vivo injection will be described as well as preliminary work on the future of these systems for coupled imaging and therapy.

Biography:

Frederic LEROUGE is a professor assistant at the University Lyon 1 working in the Chemistry laboratory of the ENS Lyon. His main research interests are the design of inorganic nanoparticles of various size and compositions together with the surface modification/ functionalization of these systems. The targeted fields of applications are optics, plasmonics, imaging and therapy. He co-authored more than 60 papers and gave more than 15 invited conferences in international congresses.

Nanocrystalline Materials for Photovoltaic Applications

Pierre Kalenga Mubiayi*
Nosipho Moloto

University of Witwatersrand, South Africa

Abstract

Nanostructured materials possess interesting properties researchers seek to overcome current technological challenges. Improving the performance of existing or new devices is

the main aim set by scientist when studying nanoparticles. Cesium lead iodide, cesium tin iodide, copper indium selenide nanocrystals were prepared via classical colloidal method and microwave assisted method. Various parameters of synthesis including the time, temperature, precursor concentration, coordinating solvent and capping agent were investigated. Their properties were studied and optimized for effective application in photovoltaic devices. Several types of solar cell devices as well as perovskite cells were prepared from thin film of synthesized nanocrystals and the evidence of photovoltaic activity was shown. The performance of fabricated devices was influenced by the structure of deposited thin films, especially the absorbing layer made of synthesized nanocrystals.

Biography:

Pierre Kalenga Mubiayi is currently Lecturer in Chemistry at University of Witwatersrand. He did his postdoctoral fellowships at University of Witwatersrand, University of Zululand, Vaal University of Technology in South Africa (2015-2018). His Research focusses on nanocrystalline materials to enhance photovoltaic activity. The study extends to nanoparticles syntheses (persovskite and other inorganic nanocrystals) and their applications in various fields including water treatment and biological applications. Several publications and awards have been obtained. Research visits and collaboration have been done with a number of partners in various countries to date (Italy, Brazil, Canada, Namibia, Cameroon, England, Ghana...).

Bioactive Supramolecular Materials

Ana Maria Carmona-Ribeiro*

University of Sõo Paulo, Brazil

Abstract

Materials based on polymers, lipids and surfactants can be especially important in drug and vaccine delivery especially when they easily combine with biomolecules, drugs and vaccines, display nanometric size and are biocompatible. Over the years we dedicated our research to prepare, characterize and determine bioactivity and biocompatibility of a variety of supramolecular materials displaying antimicrobial and/or imunoadjuvant activity. In this talk we will give a brief overview on bioactive supramolecular assemblies focusing on recently developed supramolecular nanomaterials with potential as immunoadjuvants.

Biography

Founder of the Biocolloids Laboratory at the University of São Paulo in Brazil in 1993; major interests regard the invention of novel biomimetic assemblies with antimicrobial and/or immunoadjuvant activity in vivo

Variables and Electrical Properties of $BaZrO_3$-Modified $BiFeO_3$–$BaTiO_3$ Lead-Free Ceramics

Salman Ali Khan[1*]
Tauseef Ahmed[1]
Soo Yong Choi[1]
Mingyu Kim[1]
Tae Kwon Song[1]
Myong-Ho Kim[1]
Soonil Lee[1]

[1] School of Materials Science and Engineering / Department of Materials Convergence and System Engineering, Changwon National University, Changwon, Gyeongnam 51140, Republic of Korea

Abstract

A promising lead-free piezoelectric $BiFeO_3$-$BaTiO_3$-based compound was investigated regarding the synthesis of $(Bi_{0.65}Ba_{0.35})(Fe_{0.65}Ti_{0.35})O_3$ (BFBT) ceramics to suppress formation of secondary phases, control volatilization of bismuth (Bi^{3+}) and oxygen vacancy ($V_O^{\cdot\cdot}$) concentration during the heat treatment process. Optimum sintering conditions led to high static piezoelectric coefficient (d_{33}) of 200 pC/N and dynamic piezoelectric coefficient (d^*_{33}) of 411pm/V. Moreover, the modification of $BaZrO_3$ induced lattice distortion, leading to a coexistence of rhombohedral and tetragonal phases. An appropriate amount of BZ addition improved the dielectric, ferroelectric, and piezoelectric properties of BFBT ceramics. The remanent polarization (Pr) dramatically increased from 18 μC/cm2 for pure BFBT to 25 μC/cm2 for 2 mol% $BaZrO_3$. In addition, electric field-induced strain was enhanced to its maximum value (S_{max} = 0.276%) with normalized strain (d^*_{33} = 552 pm/V) at an applied electric field of 5 kV/mm. The related defects were analyzed, and the results demonstrate that the optimum thermal treatment, appropriate dopants, relative density, phase structure and minimum oxygen vacancies concentration in BF-BT system can be used to fabricate commercially viable ceramics for high temperature applications.

Biography:

Salman Ali Khan is currently working as a Ph.D. student under the supervision of Professor Dr. Soonil Lee at Changwon National University, Republic of Korea. He received his Master (M.S./ MPhil.) degree in 2019 from the "School of Materials Science and Engineering, Changwon National University Republic of Korea". His main research focuses to investigate lead-free perovskite systems, Dielectrics and Multilayer ceramic capacitors (MLCC). He published (18) SCI research papers in well-renowned international journals also attended various National and International conferences.

Statistical Analysis of Deformation Twin Transmission Across Grain Boundaries in HCP Metals

M. Arul Kumar*
K. Dang, R. J. McCabe
C.N. Tomé, L. Capolungo

Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Abstract

A detailed statistical analysis of twin transmission (TT) across grain boundaries along the twinning shear direction, η_1! (forward) and along the direction perpendicular to both twinning plane normal and shear direction, λ, (lateral) is performed in rolled, commercial purity magnesium compressed along the rolling direction (RD). EBSD images are acquired from two different cuts: a section containing the RD and normal directions (ND) to analyze forward twin transmission (FTT); and a section with a normal at 45° to the RD and ND to capture lateral twin transmission (LTT). A recently developed automated twinning analysis software, METIS, is used to obtain the statistical correlations between deformation twins and other microstructural features by analyzing EBSD microstructures comprising thousands of grains and twins. Further, Bayesian inference is employed on the obtained statistical correlations to draw statistically meaningful conclusions. This detailed statistical analysis reveals that the TT propensity decreases with increasing grain boundary (GB) misorientation angle up to 45° and there is no bias between FTT and LTT. However, FTT is favored for misorientation angles from 45° to 55°, whereas LTT is favored from 55° to 65° interval. Further, detailed analysis of TT events combining macroscopic Schmid factor and the geometric measure *m*' helps in understanding and identifying the process of twin-pairs formation, i.e., co-nucleation versus transmission. In addition, phase-field based simulations performed to understand the role of GB characteristics on TT process suggest that TT needs not to be constrained by the alignment of the twin planes, as opposed to slip transfer.

Biography:

M. Arul Kumar is a Materials Science Scientist at Los Alamos National Laboratory (LANL). He joined LANL as a postdoctoral researcher in 2013 and later was converted as a scientist in 2017. He received his PhD in Mechanical Engineering from Indian Institute of Technology Kanpur, India in 2013. His research mainly focuses on investigation of processstructure-property relationship of materials using an integrated computational and experimental methods. He is an expert in crystal plasticity-based material models, plasticity-creep-damage, diffraction experiments and statistical analysis of microstructures. He received several awards including TMS young-professional researcher award, LANL postdoctoral research award and JENESYS fellowship.

Synthesis of Nepheline from Different Zeolites Prepared from an Aluminum Waste

Aurora López-Delgado*
Isabel Padilla
Maximina Romero

"Eduardo Torroja" Institute of Construction Science, IETcc-CSIC, Spain

Abstract

Nepheline, (Na,K)AlSiO4, is a feldspatoide mineral with excellent mechanical properties, which is used in many industrial applications, specially those relate to the manufacture of glass and ceramics. Nepheline can be obtained by thermal transformation of materials rich in Na, Al and Si as zeolites. This transformation is a complex process that is affected by several factors among others the zeolite structure, the Si/Al ratio, the water content and the extra framework cations. The different mineralogical, chemical, and structural changes occurred during the transformation of zeolite to nepheline, are principally caused by migration and/or ejection of atoms from the crystal lattice of the zeolite, causing chemical stoichiometry variations as well as expansion or contraction of the material. The objective of this paper was to study the transformation of four zeolites, Ana, NaP1, LTA and, SOD into nepheline by thermal treatment. All the zeolites were prepared through a one-step hydrothermal synthesis method, using an Al-rich waste coming from the aluminum slag milling process as the only Al source. The aluminum waste is considered hazardous because of its high reactivity in the presence of water or environmental humidity. The thermal behavior of the parent zeolites was followed by differential thermal analysis and thermogravimetric (DTA-TG). Selected temperature values were used for the treatment of the zeolite in a muffle to a fixed time. Then, the samples of nepheline obtained were studied by XRD, FESEM and FTIR and the effect of the Al-waste zeolites on the morphological and microstructural characteristics of the nepheline was determined.

Biography:

Aurora López-Delgado (Ph.D in Chemistry, Scientific Researcher at Eduardo Torroja Institute for Construction Science, IETcc-CSIC) has more than 25 years of experience in the synthesis of added-value materials such as glasses, glass-ceramics, ferrites, aluminas, zeolites, etc., using hazardous waste as raw materials. She has co-authored more than 150 scientific publications, 10 patents, and around one hundred presentations at international conferences. Her current research interest includes processing and technological characterization of industrial and mining wastes in order to develop processes to get added-value materials, and also, in the application of concentrated solar energy to high temperature processes.

Programmed Exosome Fusion For Artificial Organelles

Yoon-Kyoung Cho*

Center for Soft and Living Matter, Institute for Basic Science (IBS), Dept. of Biomedical Engineering, Ulsan National Institute of Science and Technology (UNIST), Republic of Korea.

Abstract

Despite tremendous efforts to create artificial organelles as cellular implants, their application in live cells and tissues is very few owing to the limitations in terms of delivery, cellular uptake, stability, biocompatibility, and biodegradability of the synthetic materials. The natural analogs

of nanoreactors made of biomembranes, such as exosomes, play an active role in intercellular communication and are recognized as a promising source of diagnostic biomarkers and therapeutic agents. In this study, we used exosomes as a natural compartment that allowed encapsulation of multiple exogenous reagents to facilitate enzymatic reaction within the cell. Using a supramolecular chemistry-based fusion of exosomes enabled in cell-sized droplet microreactors, we could demonstrate the controlled fusion of exosomes that act as nanoreactors for biocatalytic cascade reactions. Furthermore, we engineered the exosome membrane proteins and encapsulated multiple reagents and enzymes to form a minimal electron transport chain capable of energy generation (ATP production) for many hours after uptake into living cells. The artificial organelle made of all-natural ingredients showed efficient penetration into the core of tissue spheroids and supplied ATP and reduced ROS levels. We believe that our study makes a significant contribution to the literature because this strategy could be used to develop new biomaterials, synthetic cell networks, miniaturized bioreactors, implanted theragnostic devices, and responsive soft-matter microsystems by bridging the bottom-up synthetic biology and bio-inspired engineering area.

Biography:

Yoon-Kyoung Cho is a full professor at UNIST and a group leader at IBS, Korea. She received Ph.D. in Materials Science and Engineering from the University of Illinois at Urbana-Champaign in 1999, having obtained M.S. and B.S. in Chemical Engineering from POSTECH in 1994 and 1992, respectively. She worked at Samsung Advanced Institute of Technology before joining UNIST in 2008. She is a member of the National Academy of Engineering of Korea, an associate editor of ‘Lab on a chip’, a fellow of the Royal Society of Chemistry, and a board of directors of the Chemical and Biological Microsystems Society (CBMS).

Nanometric Chiral Platform for the Induction of Chiroptical Properties to Functional Nanoparticles/Molecules

Reiko Oda*

Univ. Bordeaux, CNRS, Bordeaux INP, CBMN, UMR 5248, F-33600 Pessac, France

Abstract

Nanometric helices with controllable pitches are attractive not only to mimic nature, but also for the wide range of applications in materials sciences, chemical and biomaterial sensing, and enantioselective catalysis. We have reported that chiral supramolecular assembly system can be achieved from non-chiral cationic surfactants with chiral counterions1. In this talk, I discuss how such structures can then be used as scaffold to obtain hybrid organic/ inorganic nanohelices,2 which can then be used as chiral platform to 1) organize chirally achiral nanoparticles or dyes3 or to 2) perform in-situ synthesis of nanometric helical metals/ quantumdots/cyristals and induce chiroptical signals from them.4 Finally, such functionalized chiral nano structures show interaction with Intrinsically chiral or pro-chiral molecules, possibly giving access to enantioselective sensors.

Biography:

Reiko Oda, after obtaining a bachelor degree in physics at the University of Tokyo in 1988, got her PhD in Physics at the Massachusetts Institute of Technology in 1994 under the supervision of Pr. D. Litster. She then had four years of postdoctoral position in the laboratory of S. J. Candau at University Louis Pasteur (Strasbourg). She joined the IECB on 1998 as a group leader. Her research deals with the structural study and design of aggregates of amphiphilic molecules and their interactions with biological polyions, as well as functionalization of such aggregates.

Mechanical Properties of Eco-Friendly Polyamide 11 Based Laminated Structures

Pietro Russo[1*]
Libera Vitiello[2]

[1]Istituto per i Polimeri, Compositi e Biomateriali, Consiglio Nazionale delle Ricerche, Via Campi Flegrei 34, 80078, Pozzuoli-Napoli, Italia

[2]Dipartimento di Ingegneria Chimica, dei MAteriali e della Produzione Industriale, Università degli Studi di Napoli Federico II, P. le Vincenzo Tecchio 80, 80125, Napoli, Italia

Abstract

In the last decades, the growing industrial demand for structures with increasingly specific performances but sustainable from both an environmental and an economic point of view pushed research towards the development of new eco-friendly materials.

In this frame, this contribution deals with the mechanical performances of laminates based on three polyamide 11 matrices: two neat but with different average molecular weight and one containing a plasticizing agent; and three fabrics: a hybrid comprising flax and basalt fibres and two fabrics with twill architecture consisting of the weaving of only flax and only basalt fibres, respectively.

A preliminary rheological investigation of the matrices allowed, among other things, to optimize the process conditions for the preparation of all the samples carried out by means of common film stacking and hot pressing procedures.

Specimens of suitable dimensions obtained from the plates of each material were systematically subjected to mechanical bending and dart fall impact tests. The results, appropriately supported by morphological investigation of the induced damage, highlighted a good combination of flexural properties and toughness for hybrid specimens. Expectedly, the presence of a plasticizer contributes to a greater deformation and energy absorption capacity of the composite but also to a slight reduction in mechanical stiffness but with tolerable effects given the significant interfacial interlocking guaranteed by the architecture of the woven fibres considered. Furthermore, the exploration of a polyamide 11 grade with a relatively low average molecular weight made it possible to significantly reduce the process temperature and, therefore, to alleviate any degradation phenomena affecting the flax fibres.

Biography

Russo Pietro, graduated with laude in Chemical Engineering at the University of Salerno (I) on 1991. His main research interests are processing technologies including recycling of polymer based formulations and nanocomposites, green polymer composites involving bio-based matrix and/or natural reinforcing fibers, polymer materials with improved functional properties, mechanical and damage behavior of composite laminated structures. In these fields he coordinated many research funded projects. Russo is co-author of 170+ publications in peer-reviewed international journals, 8 book chapters and co-editor of 1 book "Experimental Characterization, Predictive Mechanical and Thermal Modeling of Nanostructures and their Polymer Composites" - Elsevier.

Low Power Full Color Diffractive Display using Colloidal Arrays in Nonpolar Medium

Wonmok Lee[1*]
Eunsun Park[1]
Hyunjung Lee[2]

Sejong University, South Korea[1]
Kookmin University, South Korea[2]

Abstract

The increasing demands for display devices with low power consumption and outdoor readability have stimulated comprehensive research on reflective displays employing tunable photonic crystal technologies. Recently, color tuning of electrophoretic crystalline colloidal array (CCA) has been demonstrated as a promising candidate for full color reflective display. To overcome problematic features of water in electric field, non-aqueous liquid medium is required. Herein, CCA formed from core-shell PMMA/poly(t-butyl methacrylate) microspheres was fabricated, which was stabilized by the charged inverse micelles of amphiphiles in iso-paraffinic fluid. A highly charged all-organic CCA was found to exhibit full-color tunability with a thousand-fold reduction in the operating current under a voltage bias in comparison with the that in an aqueous system.

Biography:

Wonmok Lee is a full professor in department of chemistry at Sejong university, South Korea. His research area covers **photonic crys**tal materials and devices, artificial opal engineering, colorimetric sensors, and color reflective displays.

The End Day-2

Oral Presentations

Relations Between Rheological, Vicat, Calorimetric, and Compressive Strength Measurements in Metakaolin-Slag-Fly Ash Geopolymers

Sepideh Akhbarifar[1,2*]
Weiliang Gong[1]
Werner Lutze[1]
Ian L. Pegg[1,2]

[1]Vitreous State Laboratory, The Catholic University of America, Washington, DC, USA
[2]Physics Department, The Catholic University of America, Washington, DC, USA

Abstract

This work contributes to our understanding of properties of geopolymers made of three pozzolans. The flexibility to tailor geopolymer properties widens significantly when using three instead of two pozzolans. We report on early stages of geopolymerization (before and after setting) of alkali-activated slag-metakaolin-fly-ash- and slag-metakaolin pozzolans. Effects of fly ash glass particle size on materials properties were studied as well. Measurements include rheology (yield stress, plastic viscosity), initial and final setting (Vicat needle penetration), heat flow up to 21 days, and compressive strength up to 28 days. A rheological time of initial setting is introduced for geopolymers, based on measurements of yield stress and plastic viscosity. The results of needle- and rheological measurements are compared and quantitatively related to heat- and set time data. Maximum heat flow and compressive strength were found to be linearly correlated in these ternary geopolymers.

Biography:

Sepideh Akhbarifar is a postdoctoral researcher in physics-materials science and adjunct faculty in the School of Engineering at The Catholic University of America. She holds a Ph.D. in physics, has master's degrees in Nuclear Environmental Protection and in Chemical Engineering. Her interests focus on environmental protection, specifically energy efficiency and clean air. Her research comprises thermoelectric materials, metal-insulator-transitions, low-CO2 geopolymers, dust removal (advanced cyclones). She was honored as 'Young Women Inventor 2010' by Iran's National Elites Foundation. She publishes widely and holds two patents. She is a member of several scientific societies as well as member of the 'Early Career Subcommittee' of the Materials Research Society.

Quantum Defects in Two Dimensional Materials: Local-Symmetry-Guided Discovery and Design

Qimin Yan

Temple University, USA

Abstract

Being atomically thin and amenable to external controls, two-dimensional (2D) materials

offer a new paradigm for the realization of patterned qubit fabrication and operation at room temperature for quantum information sciences and technologies. In this talk, as an example of quantum material design by local bonding symmetry, I will discuss how data-driven material science can be combined with symmetry-based physical principles to guide the search for quantum defects in two-dimensional (2D) materials for quantum information processing and quantum computing. The use of local bonding symmetry (irreducible representations) as a material design hypothesis enables the identification of anion antisite defects as promising spin qubits and quantum emitters in six monolayer transition metal dichalcogenides. The work creates a technically accessible 2D platform for the fabrication of defect-based multi-qubit systems for quantum computing. At the end of the talk, I will discuss the development of graph neural network-based machine learning models that embrace attention and take advantage of self-supervised learning, which will greatly accelerate the discovery of "defect genome" in a vast space of 2D material systems.

Biography:

Qimin Yan is an Assistant Professor of Physics at Temple University. He received his Ph.D. degree in Materials from University of California, Santa Barbara in 2012. From 2013 to 2016, he was a postdoctoral researcher at Lawrence Berkeley National Lab and University of California, Berkeley. In 2016, he joined the Department of Physics at Temple University as an Assistant Professor. His current research interests include physical principle enhanced machine learning and data-driven discovery of solid-state quantum materials, quantum defects for quantum computing and information technologies, and functional semiconductors for energy conversion. He received the DOE Early Career Award in 2019 and the NSF CAREER Award in 2022.

JARVIS: a Suite of Databases, ML Models and Tools for the Investigation of Crystalline Materials

Francesca Tavazza*
Kamal Choudhary
Kevin Garrity
Brian DeCost

National Institute of Standards and Technology (NIST), USA

Abstract

The Joint Automated Repository for Various Integrated Simulations (JARVIS) is an integrated infrastructure to accelerate materials discovery and design using density functional theory (DFT), classical force-fields (FF), and machine learning (ML) techniques. To date, JARVIS consists of ≈40,000 materials and ≈1 million calculated properties in JARVIS-DFT, ≈500 materials and ≈110 force-fields in JARVIS-FF, and ≈25 ML models for material-property predictions in JARVIS-ML, all of which are continuously expanding. JARVIS-tools provides scripts and workflows for running and analyzing various simulations. The JARVIS datasets and tools are publicly available at the website: https://jarvis.nist.gov. Specific areas of focus will be discussed in detail, to exemplify applicability and scientific findings.

Biography:

Member of the scientific staff at the National Institute of Standards and Technology since 2003, currently Project Leader of the "Electronic and Functional Materials" project, MSED division. Undergraduate degree in Physics and MS in Materials Science from Universita' Statale di Milano, Italy. PhD in Physics from The University of Georgia, USA. Research focus on computational modeling, high-throughput discovery, and AI/ML investigation of solid-state material properties. Over a hundred papers published in refereed journals and twenty workshops/symposia co-organized. A member of TMS since 2013, where she is currently chair of the Computational Materials Science and Engineering committee.

Recent progress in surface protection of lightweight metals by plasma electrolytic oxidation

J. Martin[1,2*]
V. Ntomprougkidis[1,2]
C. Tousch1, A. Maizeray[1,2]
G. Marcos[1,2]
T. Czerwiec[1,2]
T. Belmonte[1,2]
G. Henrion[1,2]

[1]Université de Lorraine – CNRS, Institut Jean Lamour, Nancy (France)
[2]Université de Lorraine, LabEx DAMAS, Nancy (France)

Abstract

Plasma electrolytic oxidation (PEO) is a plasma-assisted electrochemical technology to synthesize protective ceramic-like oxide coatings on lightweight metals like aluminium, titanium and magnesium alloys. PEO process is gaining a growing interest in various industrial domains (transport, energy, medicine) to replace conventional acid anodizing processes. Indeed, PEO results in improved wear and corrosion resistance together with the use of environmentally friendly alkaline. PEO process is carried out at a voltage higher than the breakdown voltage of the growing oxide layer. Consequently, PEO coatings grow under a sparking regime leading to the gradual conversion of the processed metal to an oxide layer. The growth mechanisms of the protective PEO coatings remain complex due to the combination of both electrochemical, thermal and plasma phase reactions that simultaneously occur in a small affected volume (tens of µm3).

After briefly reviewing the main scientific principles of the PEO process including the design of the experimental set-up, the microstructural and functional aspects of the PEO coatings as well as the behaviour of the micro-discharges, the present communication will focus on new achievements into the electrical management of the PEO process. It will be particularly shown that the use of sequential PEO treatments performed by adjusting suitable tuning of the current waveform during the treatment opens opportunities for a better energetic management of the PEO process. The presented results will be discussed based on the relationships drawn between the plasma diagnostic of the micro-discharges, the morphology of the produced PEO coatings and the applied electrical conditions.

Biography:

Julien Martin joined the Lorraine University in Septembre 2010 as assistant professor. He teaches physic of material at the Ecole Européenne d'Ingénieurs en Genie des Matériaux (EEIGM) and works as researcher at the Institut Jean Lamour (CNRS). His primary research interests are in the interaction between plasma and surface of materials. Currently, he is working on the innovative Plasma Electrolytic Oxidation process as a solution for light weight metal surface protection. Before joined the Lorraine University, Julien Martin graduated from the EEIGM engineering school (2005), and then received his PhD with distinction in Physic of Material from Paul Verlaine University of Metz (2009).

Surface severe plastic deformation for improved mechanical properties and increased surface reactivity of metals

Thierry Grosdidier [1, 2]*

[1]Université de Lorraine, Laboratoire LEM 3, UMR CNRS 7239, 7 Rue Félix Savart, 57073 Metz, France
[2]LABoratoire d'EXcellence "Design of Alloy Metals for low-mAss Structures" (LABEX-DAMAS), 7 rue Félix Savart, 57073 Metz, France

Abstract

Surface treatments based on repetitive mechanical impacts generate compressive residual stresses as well as plastic deformation that generate grain refinement. This can be beneficial for improving mechanical properties and for modifying the surface reactivity. However, drawbacks such as the alteration of the surface roughness as well as chemical contaminations by tooling can also have detrimental side effects. These aspects can lead to inconsistent and misleading results while comparing the performance of surfaces. This contribution will review some recent results obtained in this framework at the LABoratory of EXcellence in metallurgy "DAMAS".

The increased surface reactivity inherited from the presence of ultrafine grains and structural defects has been used to improve the diffusion of gaseous chemical species for nidtriding or H-storage applications [1,2]. In terms of mechanical properties, both the fatigue and tribological responses have been investigated. The effect of producing surface nanostructure by severe plastic deformation - before or after precipitation aging – has been tested to improve the fatigue life of Al alloys [3]. The analysis of the tribological behavior has shown that the surface nanostructures change the oxide formation kinetics and delay the formation of a protective Fe-rich third body oxide layer on Ti [4]. These results indicate that apparently contradicting literature results can be explained by taking into account the contamination induced during the peening process.

Biography:

1. Recent developments in the application of surface mechanical treatments … , T Grosdidier, M Novelli, Materials transactions, 1344-1355, 2019.
2. Effect of gradient-structure versus uniform nanostructure on hydrogen storage …, K Edalati, M Novelli, S Itano, HW Li, E Akiba, Z Horita, T Grosdidier, Journal of Alloys and Compounds, 337-346, 2018.
3. How does surface integrity of nanostructured surfaces influence fatigue … ?, P Maurel, L Weiss, T Grosdidier, P Bocher, International Journal of Fatigue, 105792, 2020.
4. Oxide dependent wear mechanisms … , P Maurel, L Weiss, P Bocher, E Fleury, T Grosdidier, Wear, 245-255, 2019.

Photoconductivity in monolayer MoS2: Spectral behavior and physical regimes

Jorge Quereda*

Complutense University of Madrid, Madrid, Spain

Abstract

In the last 15 years the optoelectronic properties of monolayer (1L) transition metal dichalcogenides (TMDs) in general, and MoS2 in particular have been thoroughly studied due to their great potential for photodetection. In this talk I will discuss the spectral behavior of photoconductivity in high-quality monolayer MoS2 devices, measured at cryogenic temperatures and explore the different physical regimes and mechanisms responsible for photoconductivity.

Biography:

I am an experimental physicist specialized in the field of two-dimensional (2D) materials and devices. Over the last few years my research has slowly drifted from characterizing the optical, mechanical, and electronic properties of 2D materials from a fundamental perspective to developing more complex structures and devices based on these materials, aiming to explore and exploit exotic optoelectronic regimes. Since January 2022 I initiated my own research group at Complutense University of Madrid, aimed to studying nonlinear optoelectronics in low-symmetry 2D materials.

Development of graphene-containing hydrophobic antibacterial and antiviral textile coatings for self-sanitizing textile materials

Ivan Jerman[1*]
Danaja Štular[1]
Barbara Simončič[2]
Brigita Tomšič[2]
Polona Kogovšek[3]
Sivasambu Bohm[4]

[1]National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia
[2]University of Ljubljana, Faculty of Natural Sciences and Engineering, Aškerčeva 12, 1000 Ljubljana, Slovenia
[3]National Institute of Biology, Večna pot 111, 1000 Ljubljana, Slovenia
[4]Imperial College London, South Kensington Campus London SW7 2AZ, UK

Abstract

Textile fibers provide a large surface area for pathogen adherence and growth; thus, they pose a high risk for the spread of bacterial and viral infections. Taking this into consideration, the development textile materials which prevent the transmission of pathogens before they reach a new host is urgently needed. The aim of our research was to develop protective textile coatings with efficient active and passive protection against bacteria and viruses, using a new and unique approach. As active biocidal components few-layer graphene (FLG) and copper micro-flakes (CuMF) were used and incorporated into the polyurethane coating matrix. FLG is characterized by larger surface area and greater amount of edges which are key components for the biocidal activity of graphene, while CuMF were chosen because Cu nanoparticles exhibit greater cytotoxicity compared to microscopic particles. Passive protective properties

were achieved by providing low adhesion of the fibre surface, with the use of C6-fluoroalkyl functional water-born siloxane (FAS), which represents environmentally friendlier alternative to the previously widely used C8-perfluorinated compounds. The biocidal components CuMF and FLG acted synergistically and provided a strong reduction of both Gram-negative and Gram-positive bacteria with log reduction up to 9.81, and high antiviral properties, reducing bacteriophage phi6 by log >5.5. Moreover, the addition of FAS increased the water contact angles up to 144 °. Functionalised textile materials showed both passive protection due to the low surface energy, which disabled the contact of pathogens with the material, and active self-sanitising activity, which was reflected in the high reductions of pathogens.

Biography:

Ivan Jerman, PhD. (M) is a senior researcher, Head of Coating development laboratory, part of Department of Materials Chemistry, at National Institute of Chemistry. He graduated at the University of Ljubljana, Faculty of Education in 2005 and Received Ph.D. degree at the University of Ljubljana, Faculty of Chemistry and Chemical Technology in 2009. Research interest: synthesis of Polyhedral Oligomeric Silsesquioxane; sol-gel thin films; modification of pigments for spectrally selective paint coatings. High solar absorptivity coatings for concentrated solar power; textile finishing; surface treatments; nanocoatings… He published over 200 publications including over 86 refereed scientific papers in the international journals with impact factor, 2 published invited scientific conference contributions and over 100 papers presented at the international meetings and congresses and printed in the book of abstracts and a chapter in a monograph in the international scientific book. He is co-author of 2 Patent application and 7 patents. Papers are cited over 2000 times, h-index 20.

Diffusion behavior of light guest molecules and nanopores characterization of semicrystalline phases of syndiotactic polystyrene

Kevin R. Arriola-González
Alejandro Gil-Villegas
Susana Figueroa-Gerstenmaier*

Division of Sciences and Engineering, University of Guanajuato, León, Mexico

Abstract

Syndiotactic polystyrene is a semicrystalline stereoregular polymer (30-50% degree of crystallinity) which is easily crystallizable with high melting point presenting a very complex polymorphic behavior. There are two semicrystalline phases with trans-planar chains (α and β) and three with helical s(2/1)2 chains (γ, δ, and ε). Two of the helical semicrystalline phases (δ and ε) present nanopores, being able to absorb, even from diluted solutions, low-molecular-mass guest molecules in cavities of their structures, eventually leading to the formation of host-guest semicrystalline phases. The δ phase presents two identical cavities and eight styrene monomeric units per unit cell, while the ε phase, with 4 chains per unitary cell, exhibits channels parallel to the chain axes. It is worth to note that the sorption of gases (and in general of guest molecules) from polymer semicrystalline phases is a rather unusual phenomenon. The nanoporous semicrystalline phase δ has been extensively investigated but the ε phase is still almost unexplored. In this work, we present results using a geometrical method to obtain the size and shape of the channels inside the material in terms of the size of guest molecules for the semicrystalline ε phase. Diffusion behavior of light guest molecules inside of the matrix was also analyzed using molecular dynamics.

Biography:

Mexico City, 1968

Full Professor in University of Guanajuato

Chemical Engineering, UNAM, Mexico, 1990

Master's in Chemical Technology (Biotechnology) IQS, Barcelona, Spain, 1993

Master of Chemical Sciences (Physical chemistry) UNAM, Mexico, 1997

PhD in Chemical Engineering, Rovira i Virgili University, Tarragona, Spain, 2002

Stay at North Carolina State University, Raleigh, USA, 2002

Stay at the Institute of Fundamental Chemical Processes of the Czech Academy of Sciences, Prague, Czech Republic, 2003

Post-doctorate, UOIT, Oshawa, Canada, 2004-2006

Post-doctorate, University of Salerno, Italy, 2007-2009

Professor at the University of Guanajuato, since January 2010

Sabbatical year, Technical University of Darmstadt, Germany, 2016-2017

Crude oil analyst, Petróleos Mexicanos Internacional, 1991 and 1993-1994, Mexico City

Molecular modeling of adsorption processes and characterization of nanomaterials.

Calculation of thermodynamic, dynamic, and structural properties of systems of interest in Chemical Engineering.

Modeling of the biochemical processes involved in Alzheimer's.

Modeling of multi saccharides and biopolymers.

Towards a new indirect approach by vibrational spectroscopy to evaluate mechanical properties within tellurite-based glass systems

Maggy Colas[1*]
Jonathan de Clermont-Gallerande[1]
Marianne Evrard, Philippe Thomas[1]
Fabrice Célarié[2]
Yann Gueguen[2]
Michael Bergler[3]
Dominique de Ligny[3]
Tomokatsu Hayakawa[4]
Frederic Desevedavy[5]
Frederic Smektala[5]

[1]Institute of Research on Ceramics (IRCER), UMR CNRS 7315, Limoges University, 12 Rue Atlantis, 87068 Limoges, France

[2]Institut de Physique de Rennes (IPR), UMR CNRS 6251, Rennes University, 263 Avenue Général Leclerc, 35700 Rennes, France

[3]Institute of Glass and Ceramics, DMSE, University of Erlangen-Nuremberg, DE 91058 Erlangen, Germany

[4]Nagoya Institute of Technology (NITech), Gokiso, Showa, Nagoya 466-8555, Japan

[5]Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), UMR CNRS 6303, Bourgogne Franche-Comté University, 9 avenue Alain Savary,BP 47870, 21078 Dijon Cedex, France *maggy.colas@unilim.fr, +33 5 87 50 23 80

Abstract

Tellurium oxide-based glasses have great interests due to their specific physical and chemical

properties such as high refractive index, wide band infrared transmittance and large third order non-linear optical susceptibility , up to 50 times higher than silica glasses [1]. This work will focus on different kind of tellurite system, which have been choose for their potential ability to fiber shaping for specific nonlinear optical applications. In this communication, the structural properties are evaluated by using in situ temperature Raman spectroscopy, and the mechanical properties are studied using Resonance Frequency Data Analysis (RFDA) [2,3] as a function of temperature. Finally, a simultaneous investigation of thermal, structural and elastic properties has been obtain by using the ARABICA setup [4]. Thus, a new point of view on the correlation between mechanical and structural properties, and especially around Tg has been evidence. This approach could be a key point for being able to choose the best tellurite system to the optical fiber shaping by using only a vibrational approach. References [1] R. H. El-Mallawany, Tellurite Glasses Handbook: Physical Properties and Data, Second Edition. CRC Press, (2011) [2] P. Mezeix, et al, J. Non-Cryst. Solids 445-446 (2016) 45 [3] N. Ghribi PhD, Limoges University (2015) [4] A. Veber et al, Analytica Chimica Acta, 37-44 (2018) 998

Biography:

Maggy COLAS, I am CNRS researcher in the Institute of Research on Ceramic, in Limoges. My area of expertise is based on Raman spectroscopy as a tool for structural investigations within different kind of ceramic materials. The main aim is to be able to correlate the structure of materials to their physical researched properties.

Ultimate-density ferroelectric memories by flat bands in HfO2

Jun Hee Lee

Ulsan National Institute of Science and Technology (UNIST), Korea

Abstract

Since ferroelectricity is a collective phenomenon requiring the simultaneous displacement of at least thousands of atoms, it's been believed since it's discovery in 1920 that finite-sized domains (10~100nm) are required to stabilize and switch the ferroelectric dipole moments. Here, we break the 100-years belief if we introduce flat-band physics into the history of ferroelectricity. As flat energy band in momentum space has been already known to induce the localized states in real space and to cause very unusual phenomena such as graphene superconductivity and electron lattices, we discovered that, for the first time, flat bands in phonon exist surprisingly in the commercial ferroelectric HfO2 and showed that they induce irreducibly localized dipoles of a few angstroms in real space. More strikingly, these extremely localized dipoles are individually stable and switchable by external electric field and thus now one circumvents the formation of the conventional large domains for the ferroelectric dipole switching. We can directly switch the ultimately-small unit-cell-scale dipoles and finally pave a way to achieve densest memory devices by employing the fundamental flat-band physics in the most commercial ferroelectric directly compatible with Si-technology [1].

Biography:

Jun Hee Lee received his PhD from Seoul National University in 2008. He has various research experiences from his post-doctor periods at Rutgers University, Princeton University and Oak Ridge National University (2008~2015). Since 2015, he joined Ulsan National University of Science & Technology (UNIST) in Korea as an assistance professor. Now he is an associate professor working on ferroelectricity, multiferroicity and various energy materials.

Compoutational Calculations on Dry and Hydrated Molybdenum Disulfide-Graphene Heterostructures as Efficient Hydrogen Evolution Reaction Catalysts

Nicholas Dimakis[1*]
Sanju Gupta[2]
Razeen Wadud[1]
Muhammad I. Bhatti[1]

[1]University of Texas Rio Grande Valley, Edinburg, USA
[2]Pennsylvania State University, University Park, 16802, USA

Abstract

Molybdenum disulfide-graphene heterostructures (MoS2/graphene) are promising cost-effective, highly stable, efficient, and greatly active electrocatalysts for hydrogen evolution reaction (HER). We present density functional theory (DFT) electronic calculations for dry and hydrated pristine and defect MoS2/graphene under comprehensive strain. In the pristine heterostructure, a small bandgap (minigap) is opened at the graphene Dirac point, which is located above the Fermi energy, for dry and hydrated configurations. The presence of sulfur and carbon vacancies in the MoS2/graphene upshifts the Dirac point and widens the minigap. Increased sulfur vacancies further widen or shrink the minigap depending on the location of the MoS2 conduction band bottom and the presence of defect bands at the Dirac point. The minigap tunability in the MoS2/graphene heterostructure could be engineered for producing efficient HER electrocatalysts and beyond. The Quantum Theory of Atoms in Molecules (QTAIM) reveals S-C bond critical points, which correspond to van der Waals forces interactions in agreement with the Non-covalent Interaction (NCI) analysis. We draw a correlation between the minigap and the electron density at the S-C bond critical points.

Biography:

Nicholas Dimakis is a Full Professor and Department Chair at the University of Texas Rio Grande Valley. He graduated with a Ph.D. in Physics from Illinois Institute of Technology (IIT) in Chicago and worked at the IIT collaborative accesses team at the Advanced Photon Source beamline for several years before joining UT Pan-American as Assistant Professor in 2004. His research is on computational material science applicable to a variety of materials such as platinum-based alloys, heterostructures, and pyrochlores. He has about 52 peer-reviewed publications and participated in externally funded grants of about $8M.

In situ Formation of High Thermal Expansion Composite from Pyrex-Type Glass

Jacob Hormadaly

Ben-Gurion University,Israel

Abstract

Barium silicates have been investigated as high expansion components of solid oxide fuel cells (SOFCs) and therefore their synthesis and expansion were the subject of intensive research in recent years. In this presentation we briefly present two novel findings related to synthesis rout of sunbornite (BaSi2O5) and fast in-situ formation of high expansion sunbornite composite from Pyrex-type glass powder. Low temperature synthesis, composition and

expansion of novel glass composites are described. The composites are made by the reaction of $BaCO_3$ and Pyrex-type powders at 850-950°C for a short time of one hour. Composites are well sintered, hard and their linear coefficient of thermal expansion is about $12.3 \times 10^{-6} C^{-1}$. Crystalline phase formation , dilatometer measurements , SEM data and possible applications of the composites are presented and discussed .

Reconfigurable Photonic Crystals and Chromogenic Sensors Enabled by Multistimuli-responsive Shape Memory Polymers

Peng Jiang

Department of Chemical Engineering, University of Florida, Gainesville, FL 32611

Abstract

Smart shape memory polymers (SMPs) can memorize and recover their permanent shape in response to an external stimulus, such as heat, light, and solvent. They have been extensively exploited for a wide spectrum of applications ranging from biomedical devices to aerospace morphing structures. However, most of the existing SMPs are thermoresponsive and their performance is hindered by heat-demanding programming and recovery steps. By integrating scientific principles drawn from two disparate fields − the fast-growing photonic crystal and SMP technologies, we have developed a new type of SMP that enables unusual "cold" programming and instantaneous shape recovery triggered by applying a large variety of stimuli, such as static pressure, shear stress, laser, microwave, solvents, and vapors, all at room temperature. This interdisciplinary integration simultaneously provides a simple and sensitive optical technique for investigating the intriguing shape memory effects at nanoscale. We have also demonstrated the fabrication of reconfigurable nanooptical devices, such as photonic crystal filters and chromogenic sensors, as well as tunable antireflection coatings, using these new multi-stimuli-responsive SMPs. The striking chromogenic effects induced by the unusual shape memory behaviors of the smart polymers provide vast opportunities for a plethora of applications ranging from reconfigurable nanooptical devices to chromogenic pressure and chemical sensors to novel biometric and anti-counterfeiting materials.

Biography

Jiang is a full professor in the Department of Chemical Engineering at the University of Florida. He obtained Ph.D. from Rice University and was a postdoctoral fellow at Princeton University. He worked at Corning and GE for a few years before he started his academic career. His current research interests include material self-assembly, shape memory materials, scalable nanomanufacturing, and biomimetic materials. Dr. Jiang has published more than 100 peer-reviewed papers with over 12,000 citations in prominent journals, such as Science and Nature Photonics. He was the recipient of the prestigious NSF CAREER Award.

Stimuli-Responsive Janus Emulsions

Joachim Koetz

University of Potsdam, Germany

Abstract:

Stimuli-responsive Janus emulsions consisting of two non-mixable oil components, i.e.

olive oil (OO) and silicone oil (SiO), prepared by a moderate energy vibrational route, have attracted reinforced research interests due to their tuneable optical, magnetic, pH- and thermo-responsive properties. By using an amphiphilic copolymer of 2-(meth-acryloyloxy) ethyl oleate and N,N-diethylacrylamide as emulsifier, a temperature dependent "explosion" of Janus droplets can be triggered at 35 °C due to the collapsed polymer at the interface [1]. When chitosan-stabilized Janus droplets are used one can tune the droplet size by varying the pH value. By adding magnetite nanoparticles the droplet size can be decreased and superparamagnetic properties can be imported [2]. This offers a way to produce ultralight magnetic aerogels after freeze drying [3]. Surprisingly, gold nanoparticles can stabilize Janus droplets, too. The resulting Pickering Janus emulsions show special optical effects with a multitude spectrum of coloured rings. Furthermore, incorporated magnetite nanoparticles allow a rotation of the inner oil SiO droplet by stimulation in an external magnet field.

Biography:

Joachim Koetz studied chemistry at the Martin-Luther University Halle/Wittenberg and obtained his Ph.D. in Polymer Chemistry under supervision of Burkart Philipp in 1986 from the Institute of Polymer Chemistry of the Academy of Science in Teltow-Seehof (Germany). In 1992 he received habilitation and since 1994 he has been Professor of Colloid Chemistry at the University of Potsdam. His main interests are nanoparticles, polyelectrolytes, liquid crystalline systems and microemulsions. He published more than 220 papers (h-index: 31; including 2 books and above 10 book chapters), 11 patents, and gave more than 120 oral presentations at conferences.

Inside Polymers: Unravelling Polymer Structure and Dynamics With Neutrons

Mariela Nolasco

University of Aveiro, Portugal

Abstract

This work aimed at the characterization of polymer structure and dynamics. These embraces both natural polymers (e.g. cellulose and bacterial cellulose) and bio-based synthetic polymers (furandicaboxylate polyesters). The main strategy to delve deeper into the structure−property correlations in polymeric materials takes advantage of inelastic neutron scattering (INS) combined with discrete and periodic DFT calculations. This combination is ideal either to assist the elucidation of measured data or, conversely, as method of validating theoretical models. In particular, the synergy between INS and CASTEP calculations allowed the reliable assignment of INS bands to vibrational modes of crystalline polymer forms. In the case of furandicaboxylate polyesters, discrete DFT calculations on model systems predicted the spectral patterns to be found for amorphous regions.

Biography:

Mariela Nolasco (b. Barquisimeto, VE) works as a Research Assistant at Chemistry Department/ University of Aveiro in the subfield of Physical Chemistry. Her research interests encompass the combined use of computational methods (discrete DFT/TD-DFT and periodic CASTEP) and spectroscopic techniques (Photoluminescence, FT-IR, Raman and Inelastic Neutron Scattering) to bridge the gap between the theory and the experiment. She has co-authored more than 44 scientific articles, 1 book chapter and several communications at scientific meetings. She is a competitive researcher that was the PI of 8 R&D international short-term projects at neutron facilities at ISIS Neutron & Muon Source and Institut Laue-Langevin.

Morphology of Graphene Flakes in Ni-Graphene Nanocomposites and its Influence on Hardness

Vardan Hoviki Vardanyan[1]
Herbert M. Urbassek

[1]Physics Department, University Kaiserslautern, Erwin-Schrodinger-Straße, D-67663 Kaiserslautern, Germany andResearch Center OPTIMAS, University Kaiserslautern,ErwinSchrodinger-Straße, D-67663 Kaiserslautern, Germany

Abstract

We investigate the effect of graphene flakes on the strength of Ni-graphene composites using molecular dynamics simulation. Flakes are inserted into the heated liquid Ni and the structures are equilibrated in a 14-ns molecular-dynamics run. By varying the interaction of flake edge atoms with the Ni matrix, two different flake morphologies – wrinkled vs flat – are obtained. We studied the effect of the morphology of graphene flakes in a Ni-graphene nanocomposite on the mechanical properties, in particular the hardness. The high concentration of graphene in the plastic zone of the nanoindenter leads to a strong absorption of dislocations. Some of the dislocations present by the solidification process before the indentation were annihilated. However, this effect only occurs for the wrinkled flake morphology; there, the absorption of dislocations at the flake dominates the pile-up and leads to a strong reduction in hardness, amounting to roughly 10 % in the case investigated. No effect of the changed interaction between graphene edge atoms and the Ni matrix on the dislocation activity and hardness could be observed. Furthermore, we demonstrate that a high graphene content in the plastic zone leads to an increased dislocation absorption and weakens the composite.

Biography:

I was born in Armenia in 1989. I graduated from Yerevan State University(2010), with bachelor degree in physics. Next I completed my military service (2012) and moved to Israel to continue my study. I obtained scholarship in Ben-Gurion University, majoring in computational physics (2015). My master project was on mean-field model of electrical double layer. I pursued my doctoral degree in TU Kaiserslautern, Germany (2017). My current doctoral project centers on molecular dynamics simulation of plastic deformations occurring in composite materials. My research contributions have been to investigate hardening mechanisms in graphene metal matrix composites and brittle-ductile interfaces.

Using Photons for Materials Processing

Julia W. P. Hsu*
Weijie Xu
Robert Piper

Department of Materials Science and Engineering, University of Texas at Dallas

Abstract

Annealing using hot plates or ovens is a common method to stimulate chemical reactions or phase transformation in materials, to remove remnant reactants or solvents, or to improve

a material's crystallinity or electrical properties. However, it posts insurmountable challenges when making metal oxide films on flexible substrates such as paper or plastics: the high temperatures needed to convert or activate metal oxides can damage the low-temperature substrate materials and the drastically different coefficient of thermal expansion (CTE) of the film and the substrate would lead to mechanical failures in the brittle oxide films. Photonic curing uses short pulses (25 μs to 100 ms) of broadband (200 – 1500 nm) light from a xenon flash lamp to deliver energy to the sample. The energy is preferentially absorbed by the film, leading to selective heating of the film while the substrate remains cool, hence avoiding damaging the substrate or causing thermal stress in the film from CTE mismatch. Furthermore, because the light pulses are short, even though the intensity is high, the total energy absorbed by the sample is low. In this talk, I will discuss how we use photonic curing to fabricate metal oxide and halide perovskite films for flexible capacitors and organic-inorganic halide perovskite solar cells.

Biography:

Julia W. P. Hsu is Professor of Materials Science and Engineering at the University of Texas at Dallas and holds the Texas Instruments Distinguished Chair in Nanoelectronics. Her work has covered diverse fields of materials, including superconductors, epitaxial inorganic semiconducting films, metal oxides, polymer and organic semiconductors, and organicinorganic halide perovskites for energy, environment, and electronic applications. Dr. Hsu is a Fellow of the American Physical Society (APS), the American Association for the Advancement of Science (AAAS), and the Materials Research Society (MRS).

Microwave and Molten Salt Co-assisted Synthesis of Boron-containing Ceramics

Shaowei Zhang[1*]
Cheng Liu[1]
Haijun Zhang[2]
Liang Huang[2]
Jianghao Liu[2]

[1]University of Exeter, UK
[2] Wuhan University of Science and Technology, China

Abstract

Because of their superior properties such as high melting point, high mechanical strength, excellent wear resistance, and outstanding chemical resistance, boron-containing ceramics are used extensively at both low and high temperatures in many important sectors, including armour, aerospace, machinery, thermal management, refractories, and nuclear reactors.

Numerous techniques have been used to prepare boron-containing ceramics. Unfortunately, they suffer from various disadvantages, in particular, requirement of high synthesis temperature, use of expensive raw material precursors and heavy agglomeration of product powder.

To address these issues, the present authors have developed a novel microwave and molten salt co-assisted synthesis strategy, and prepared a range of binary and ternary boron-containing ceramic powders, including ZrB_2, HfB_2, TiB_2, $Al_8B_4C_7$, MoAlB, TiB_2-$MgAl_2O_4$, TiB_2-TiC, and ZrB_2-SiC. Following these successes, several emerging high-entropy boride ceramic powers, e.g., $(Hf_{0.2}Ti_{0.2}Mo_{0.2}Ta_{0.2}Nb_{0.2})B_2$, and $(Hf_{0.167}Zr_{0.167}Ti_{0.167}Ta_{0.167}Nb_{0.167}V_{0.167})$

B2, have been further synthesized. The synthesis temperatures generally can be reduced by several hundred degrees, compared to those required by the conventional synthesis techniques. Moreover, morphologies and sizes of the product powders can be readily tailored/ controlled. In most cases, well-dispersed nanosized or submicron sized product powders can be obtained, guaranteeing the excellent properties of the final bulk ceramic counterparts. The above promising results are attributable to the molten salt medium under microwave heating, which facilitate the reaction processes via two main mechanisms, “dissolution–precipitation” and “template growth”.

In addition, some important properties of the synthesized ceramics (e.g., the high-entropy boride ceramics) have been predicted by Density functional theory (DFT) calculations, and compared with the experimental results.

Biography:

Shaowei Zhang is currently full professor and Royal Society Industry Fellow at University of Exeter, UK. He is also a Fellow of Institute of Materials, and Royal Society of Chemistry. Before moving to Exeter, he had worked at University of Sheffield as Lecturer and Reader. His main research interests are in the processing, characterization and applications of advanced ceramics. Prof. Zhang has published over 350 refereed journal papers, and authored/co-authored 8 books and book chapters. He is the editor of “Refractories Manual”, a guest editor of “Materials”, and an associate editor of Journal of American Ceramic Society.

The End Day-3

Virtual Presentations

Identification of Solids for True Design and Precise Characterization of Functional Materials

Bunsho Ohtani*
Mai Takashima

Institute for Catalysis, Hokkaido University, Sapporo 001-0021, Japan

Abstract

How can we design solid materials such as catalysts and photocatalysts? What is the decisive factor controlling those materials' performances/activities? So-called band-structure model (BSM), electrons in a valence band (VB) of a photocatalyst is photoexcited to a conduction band (CB), leaving positive holes in VB, and electrons and holes reduce and oxidize, respectively, substrates adsorbed on the surface of the photocatalyst, does suggest preferable band positions for redox reaction uniquely decided only by crystalline structure. The other possible factors, e.g., particle size and surface structure, cannot be discussed within BSM. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved density of electron traps (ERDT) [1,2]. Those electron traps (ETs) seem to be predominantly located on the surface of almost all the metal oxide particles, with exception of nickel oxide and therefore they reflect macroscopic surface structure in ERDT patterns. Using ERDT pattern with the data of CB-bottom position (CBB), i.e., ERDT/CBB patterns, it has been shown that metal oxide powders can be identified without using the other analytical data such as X-ray diffraction patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples can be quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. In this talk, a novel approach of material design based on the ERDT/CBB patterns is introduced [3].

[1] Chem. Commun. 2016, 52, 12096-12099. [2] Electrochim. Acta 2018, 264, 83-90.[3] Catal. Today 2019, 321-322, 2-8.

Biography:

The research work on photocatalysis by Professor Ohtani started in 1981 in Kyoto University. Since then, he has been studying material science for 40 years and published more than 300 original papers (h-index: 72). After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Graduate School of Science, Hokkaido University and was then awarded a full professor position in Institute for Catalysis, Hokkaido University in 1998. He was awarded several times from the societies related to chemistry, photochemistry, electrochemistry and catalysis.

Keynote Presentations

Extension of the ILG Mechanics Framework: Heat, diffusion and Chemical Reaction.

Elias C. Aifantis

Emeritus Professor at Aristotle University of Thessaloniki, Thessaloniki, Greece

Emeritus Professor at Michigan Technological Institute, Houghton, Michigan, USA

Mercator Fellow at Friedrich-Alexander University/Germany

Abstract

The ILG (Internal Length Gradient) Mechanics framework whose origin goes back in the mid 1980s, has been successfully applied to revisit elasticity and plasticity theories across materials and scales. Recently it has been extended to include heat conduction, mass diffusion and chemical reactions. This extension is reviewed and pertinent applications to advanced technology and biology are discussed.

Biography

Elias C. Aifantis is currently an Emeritus Professor of Mechanics at Aristotle University of Thessaloniki/Greece and Michigan Technological University/USA, as well as Mercator fellow at Friedrich-Alexander University/Germany and a Distinguished Professor at Beijing University of Civil Engineering and Architecture/China. Formerly, he has also been a Distinguished Faculty Advisor at King Abdulaziz University/Saudi Arabia, Distinguished Visiting Expert at ITMO University/Russia and Southwest Jiaotong University/China, as well as MegaGrant Director at Togliatti State University /Russia. He has promoted highly interdisciplinary work in mechanics of materials by bringing into the field of solid mechanics ideas from diffusion theory, chemical reactions, and nonlinear physics. He has coined the terms dislocation patterning, material instabilities, gradient plasticity/elasticity, chemo/nanomechanics, and pioneered internal length gradient (ILG) theories in these fields. Currently, he is extending the ILG framework to revisit electromagnetism and Maxwell's equations, as well as gravitation and Newton's Law. He has published over 350 articles and received about 13,402 citations with 59 h-index (Scopus); 12,450 citations with 55 h-index (Web of Science); 20,580 citations with 70 h-index (Google Scholar). He is included in the ISI Web of knowledge list of the world's most highly cited authors in engineering.

Oral Presentations

Towards a MEMS-Based Mechano-Acoustic Probe for Soft Tissue Characterization

Hardik J. Pandya*
Arjun B S

Indian Institute of Science, Bangalore, India

Abstract

The mechanical behavior of biological tissues has gained recent interest as the alterations in tissue properties reflect the underlying pathology and provide insights into disease progression. Recent studies have correlated mechanical responses of biological specimens to diseases and other biological mechanisms. Hence, characterizing the mechanical properties

of the tissues can be of significant prognostic value to clinicians. In this regard, the mechanical characterization of soft tissue samples such as the brain, breast, arteries, and cancers has several challenges owing to their significantly less stiffness than the engineering materials, limiting the use of many commercial tools for characterization. Also, popular nano-indentation tools are all benchtops, making their application restricted to ex-vivo characterization. Hence, there is a clear requirement of tools that can be used for in-vivo characterization of soft tissues and during a surgical setting.

Microelectromechanical systems (MEMS)-based sensors and transducers can be integrated onto low-form factor devices for various biomedical applications. The current work reports the development of a probe integrated with MEMS-based microforce sensors and piezoelectric micromachined ultrasound transducers (pMUTs) for the mechano-acoustic characterization of soft tissues. The simultaneous mechanical and acoustic characterization provides insights into the time-independent and time-dependent mechanical behaviors of the soft tissues. The characterization further helps in obtaining insights into the heterogeneity, composition, and anisotropy of soft biological specimens of scientific value. After studying the probe's performance using ex vivo tissues and larger animal models, we envisage using this probe for clinical applications in an in-vivo intraoperative setting.

Biography:

Hardik J. Pandya is an Assistant Professor at Electronic Systems Engineering (DESE), Indian Institute of Science (IISc), Bangalore. Before joining IISc, he worked as a postdoctoral scientist in the Department of Mechanical Engineering, Maryland Robotics Center University of Maryland, College Park, and in the Department of Medicine, Brigham and Women's Hospital–Harvard Medical School. He obtained his Ph.D. from the Indian Institute of Technology Delhi. His research focuses on minimally invasive and non-invasive technologies for cancer diagnosis (brain, breast, and neck), e-nose (breast cancer and chronic liver disease), and neuroprotective therapies for acute stroke and epilepsy. He has published around 50 peer-reviewed papers and has been an inventor on fourteen patents.

0-D-2 Composites of TiO2 Spheres Coupled with Graphitic C3N4 Nanosheets for Removal of olatile organic compounds

Said Al Mamari[1*]
Faisal Al Marzouqi[2]
Abdulrahman Al Nabhani[3]
Younghun Kim[4*]
Rengaraj Selvaraj[1*]

[1]Department of Chemistry, College of Science, Sultan Qaboos University, P.O. Box- 36, P.C. 9 123, Al-Khoudh, Muscat, Oman

[2]Department of Engineering, International Maritime College Oman, P. O. Box- 532, PC-322, 11 Falaj Al Qabail, Suhar, Oman

[3]Department of Pathology, College of Medicine and Health Sciences, Sultan Qaboos University, 13 P.C. 123, Al- Khoudh, Muscat, Oman

[4]Department of Chemical Engineering, Kwangwoon University, Seoul 139-701, Republic of Korea

Abstract

The different metal oxide of 0-dimitional TiO2 hollow spheres were coupled with 2-D graphitic carbon nitride g-C3N4 nanosheets to develop TiO2/g-C3N4 composites. The materials have

been fabricated by solvothermal method with different ratios. The effect of coupling was investigated by several instrumental techniques such as; X-ray diffraction (XRD), scanning electron microscopy (SEM), transmitted electron microscopy (TEM), elemental mapping, X-ray photoelectron spectroscopy (XPS), UV diffuse reflectance spectroscopy (UVDRS) and Photoluminescence (PL). The prepared composites exhibited an improvement in the visible light harvesting and reducing in the electro-hole recombination rate. In addition, the photocatalytic activity of all prepared samples was examined in the degradation of VOCs (toluene and methyl tetra butyl ether (MTBE)). About 90% of the degradation procedure were achieved due to the high interaction between the surface of TiO2 and the g-C3N4 nanosheets. Moreover, a Z-schemes of the photodegradation process and mechanism were proposed.

Biography:

Name: Said Abdullah Sulaiman Al Mamari

Date of birth: 13/12/1980

Study:

-Bachler degree form Sultan Qaboos University 2003.

-MSc degree in Chemistry from UAE University 2016.

-PhD student at Sultan Qaboos University (now).

Surface Pyroelectricity and Piezoelectricity of Centrosymmetric Crystals

David Ehre[*1]
Shiri Dishon[2]
Elena Meirzadeh[1,2]
Meir Lahav[1]
Igor Lubomirsky[1]

[1]Weizmann Institute of Science, Rehovot, Israel

[2]Department of Chemistry, Columbia University, New York, NY, USA

Abstract

Polarity, i.e., spontaneous surface charge, is usually associated with the 10, polar, out of 32 existing crystallographic classes. However, all surfaces, including those delineating centrosymmetric crystals, are inherently polar, i.e., the directions toward and outward the surface are never equivalent. This allows for a fundamental possibility for crystals, even for those belonging to the non-polar classes, to have a near surface polar layer (NSPL) arising from local symmetry reduction. The existence of such layers was only recently demonstrated, as the advances in pyroelectric1-3,5 and piezoelectric4-5 measurement techniques made them sensitive enough for the task. Piezoelectricity is the ability of dielectric materials to develop electric polarization when subjected to mechanical stress (direct effect) or change their dimensions as a result of application of an external electric stimulation (converse effect). As opposed to piezoelectricity that exist in non-centrosymmetric dielectrics, only polar materials can exhibit pyroelectricity, i. e., develop surface charge due to temperature change.In this presentation, I show that pyroelectric measurement carried out with periodic temperature change protocol (modified Chynoweth) might be a primary tool to study NSPL. Two fundamentally different examples are considered. (i) NSPL in alpha-glycine crystals develops as a result of solvent incorporation, e.g., water. This layer is maybe tens or even hundreds of

micrometers thick, sometimes, thick enough to allow piezoelectric measurements. (ii) NSPL in SrTiO3 results from surface relaxation and it is only a few Angstroms to few nanometers thick. Nevertheless, NSPL in SrTiO3 has a polarization comparable with strongly ferroelectric materials, tens of μC/cm2

Biography:

1. Piperno, S. et al. Water Induced Pyroelectricity from Non-Polar Crystals of Amino Acids. Angew. Chem. Int. Ed. 52, 6513 –6516, (2013).
2. Meirzadeh, E. et al. Nonclassical Crystal Growth as Explanation for the Riddle of Polarity in Centrosymmetric Glycine Crystals. J. Am. Chem. Soc. 138, 14756-14763, (2016).
3. Meirzadeh, E. et al. Surface Pyroelectricity in Cubic SrTiO3. J. Adv. Mater. 31, (2019).
4. Dishon, S. et al. Surface Piezoelectricity and Pyroelectricity in Centrosymmetric Materials: A Case of α-Glycine. Materials 13, 4663, (2020).
5. Meirzadeh, E. et al. Surface Pyroelectricity and Piezoelectricity of Centrosymmetric Crystals, Isr. J. Chem. 61, (2021).

Unsaturated Silsesquioxanes as Building Blocks of Novel Hybrid Systems

Beata Dudziec*
Katarzyna Mituła
Monika Rzonsowska
Julia Duszczak
Aleksandra Mrzygłód

Faculty of Chemistry and Centre for Advanced Technologies, Adam Mickiewicz University in Poznan, Poland

Abstract

Silsesquioxanes (SQs) - a family of nanosized molecular hybrid (inorganic-organic) frameworks, among which the most important are the cubic-type, i.e., T8 derivatives and recently doubledecker silsesquioxanes. Due to the nature of their defined construction that affects resulting physicochemical properties (enhanced thermal and mechanical stability, oxidation resistance, low dielectric features, hydrophobicity, etc.), they may be found in a wide range of applications. The continuous interest in the chemistry of functionalized silsesquioxanes and their appliance is a derivative of not only a few types of cores of diverse architecture but most of all the variety of reaction organic moieties that may be attached to it. The kind of organic functionalities at the Si-O-Si core is its immanent feature, which affects the type of modification to which they may be subjected. The catalytic protocols are of special importance because of their effectiveness and selectivities, e.g. hydrometallation, coupling or click processes, Friedel-Crafts, etc. Also, as the inorganic core is the scaffold for the different amounts of reactive moieties may result in the formation of various structures of resulting hybrid materials, i.a. grafted polymers, cross-linked systems, or 3D networks. They may exhibit interesting physicochemical features, which imply directions of their application. This presentations reports on the studies on the formation of silsesquioxane-based systems – precursors of hybrid materials that result from unsaturated SQs precursors. Interestingly, in some aspects, the results of those modifications may be quite unexpected.

Biography:

Beata Dudziec graduated from Adam Mickiewicz University in Poznan, Poland in 2004 and did her PhD in 2008. In 2018 she obtained his habilitation degree for research studies on functionalized silsesquioxanes. She has started her independent small research group since then. Her scientific interests concern catalytic transformations of organosilicon and organogermanium compounds and especially their specific Si-O-Si frameworks, i.e. silsesquioxanes and features of resulting molecular and macromolecular hybrid type systems.

Morphology and Structure of Al2O3-Graphene Composite Coatings Prepared by Sol-Gel Method

Bozena Pietrzyk *
Sebastian Miszczak
Bartlomiej Januszewicz
Mariusz Dudek
Lukasz Kolodziejczyk

Lodz University of Technology, Institute of Materials Science and Engineering, Poland

Abstract

In recent years, graphene and its derivatives (GO and rGO) have been of interest, also as components of composites. They can be used to modify the properties of composites in many aspects such as mechanical, electrical, anti-corrosion etc. The structure and properties of graphene also allow it to be used as a solid lubricant that reduces friction and wear. However, the effectiveness of the friction reduction mechanisms depends on the quantity, size, shape and spatial orientation of the graphene flakes. These parameters can be controlled by using graphene in composite coatings where it is a triboactive component held at the frictional contact surface by a coating matrix.

In the presented work, nanocomposite Al2O3-graphene coatings were produced by the sol-gel method. Scanning electron microscopy (SEM), atomic force microscopy (AFM), Raman spectroscopy and X-ray diffraction (XRD) were used to characterize the coatings. The morphology and structure of the coatings depending on the size and shape of the applied graphene nanoplatelets and the annealing temperature were described. It has been shown that deposition of coatings with the dip-coating method may lead to the arrangement of graphene nanoplatelets parallel to the substrate. The relationship between microstructure and tribological properties of the coatings was indicated. Changes in the structure of graphene in the alumina matrix as a consequence of the annealing temperature were also shown. The obtained results indicate the potential use of the Al2O3-graphene composites produced by the sol-gel method as ceramic coatings with a low coefficient of friction.

Biography:

Bozena Pietrzyk is a professor at Institute of Materials Science and Engineering of the Lodz University of Technology, Poland. Her research interests include methods of producing thin coatings of ceramic materials, such as sol-gel or hybrid plasma-assisted sol-gel methods. She conducts research on functional properties of ceramic and composite coatings, such as anticorrosive, antibacterial, photocatalytic and antifriction properties. She is an author and co-author of over 60 scientific journal articles and numerous conference announcements and presentations. She is an academic teacher and coordinator of two study programs. She is also a member of Materials Science Societies.

Metamaterial or Active Matter Agent Properties Induced by Interactions Between Electromagnetic Waves and Materials Suspended in a Liquid

Alain Celzard[1*]
Alexander Zharov[1,2]
Vanessa Fierro[1]

[1]Université de Lorraine, CNRS, IJL, Épinal F-88000, France

[2]Institute for Physics of Microstructures, Russian Academy of Sciences, Nizhny Novgorod 603950, Russia

Abstract

In this talk, we report some recent work on different effects produced by the interaction between electromagnetic waves and particles of various compositions suspended in a fluid.

For example, we experimentally demonstrate the controllable transmission of an electromagnetic wave through a plasmonic liquid metacrystal in the optical frequency band. We also propose the design of fully dielectric isotropic micro- or nanoparticles which, when used as structural elements of a liquid metamaterial, can simultaneously provide negative effective electrical permittivity and negative magnetic permeability. We then consider the scattering of a plane electromagnetic wave on a cylindrically inhomogeneous distribution of meta-atoms in a liquid metamaterial. The inhomogeneity of the distribution that appears following the application of an electric potential means that the effective permittivity can become negative in a certain region of space, giving rise to effects such as resonant absorption, resonant scattering, which can be controlled in real time by modifying the applied electric potential and thus reorganizing the liquid. We will also describe particles proposed as new active matter agents, self-propelled by magnetohydrodynamic acceleration of the surrounding fluid when resonantly excited by an electromagnetic wave. Finally, if time permits, the concept of light-induced movement of particles in a fluid will be extended to the development of a new method for separating chiral nanoparticles.

Biography:

Alain Celzard graduated in chemical physics in 1992 and received his PhD in materials science in 1995 in Nancy (France). Since 2005 he is full professor at ENSTIB engineering school (Epinal, France). In 2010, he was appointed Junior member of the Institut Universitaire de France. His scientific interests deal with disordered, porous and related materials, ranging from composites and nanoporous adsorbents to macroporous solid foams for catalytic, environmental, energy, or electromagnetic applications.

Ultrafast Bubble Bursting by Superamphiphobic Surfaces

Katharina I. Hegner[1*]
William S. Y. Wong[1]
Doris Vollmer[1]

[1]Max Planck Institute for Polymer Research, Mainz, Germany

Abstract

The formation and accumulation of bubbles and foams challenge a wide variety of industrial applications ranging from the food processing and commercial cosmetic sector, to electrocatalysis and flotation processes in mineral mining and waste-water treatment. If

uncontrolled, this can result in product losses, equipment downtime or damage and cleanup costs. Passive, surface-induced rapid bubble bursting and anti-foaming without the need for chemical additives are highly desirable. Here, we demonstrate how the speed of bubble bursting can be controlled via the surface morphology.1 Superamphiphobic coatings are prepared using liquid flame spray which allows simultaneous tuning of nano- and microscale structures. We identify the parameters required to achieve ultrafast bubble bursting: the nanoprotrusions should be as small as possible (diameters below 100 nm) and assembled into rough microscale features. By optimizing the surface morphology, bubble bursting can be induced within 2 ms in water. The released air is absorbed by the Cassie-state's plastron layer. The coatings demonstrate long-term ultrafast bubble rupturing and chemical and mechanical stability even in the presence of surface-active species. Furthermore, superamphiphobic surfaces are able to increase defoaming rates and inhibit foam formation. Figure 1. a,b) Side-view SEM images of particulate superamphiphobic structures prepared by liquid flame spray (scale bars are a) 20 μm and b) 1 μm). c) Images acquired by a high-speed camera show a single air bubble rupturing immediately upon contacting the surface in water (scale bar is 1 mm). References 1. Hegner, K.I., Wong, W. S. Y., Vollmer, D. Ultrafast Bubble Bursting by Superamphiphobic Surfaces. Adv. Mater. 33 (2021) 2101855.

Biography

Katharina Hegner studied Chemistry at RWTH Aachen University, Germany and received her master's degree in 2019. She joined the group of Doris Vollmer at the Max Planck Institute for Polymer Research for her master's thesis in 2018. During her PhD her research focusses on the synthesis and characterization of functional surfaces prepared via liquid flame spray. Currently, she investigates the influence of surface morphology on the nano- and micrometer scale on the surface's wetting properties.

Super Liquid Repellent Surfaces for Anti-Foaming

Doris Vollmer*
Katharina Hegner
Abhinav Naga
Lukas Hauer
Hans-Jürgen Butt
William Wong

Max Planck Institute for Polymer Research, Germany

Abstract

Wet and dry foams are prevalent in many industries, ranging from the food processing (dairy, sugar and beverage) and commercial cosmetic sectors (soaps and detergents) to industries such as chemical and oil-refining. In many chemical formulations, foaming limits the processing speed. Uncontrolled foaming results in product losses, equipment downtime or damage and cleanup costs for spillages. To speed up defoaming or enable anti-foaming, liquid oil or hydrophobic particles are usually added. However, such additives may need to be later separated and removed for environmental reasons and product quality. I will show that passive defoaming or active anti-foaming is possible simply by the interaction of foam with chemically or morphologically modified surfaces (1). Therefore, we tested superamphiphobic, liquid-infused and liquid-like surfaces using beer and aqueous soap solutions as model systems. Superamphiphobic surfaces are able to increase defoaming rates and inhibit foam

formation (anti-foaming). Up to 50% improvement in defoaming against highly stable wet foams is demonstrated. This improvements was quantified by monitoring the height of foam, the evolution of bubble numbers, radii, and coalescence-bursting events. In flotation, the use of superamphiphobic surfaces in a test setup increased material collection efficiency by 25 times. Microscopic imaging reveals that amphiphobic nano-protrusions directly destabilize contacting foam bubbles (2). Bubbles burst and the released gas escapes through the Cassie-state's air-gaps. Interfacial destabilization of foam presents a new pathway for static defoaming and dynamic anti-foaming.

(1) W. Wong et. al, Nature Communications (2021)12:5358, DOI: 10.1038/s41467-021-25556

(2) K. Hegner et. al, Advanced Materials (2021), 2101855, DOI: 10.1002/adma.202101855

Biography:

My scientific background is in physical chemistry. For many years I investigated structural and thermodynamic transitions in microemulsions, polyelectrolytes and colloids. For the last 10 years, my research has been mainly concerned with fundamental and applied problems in the wetting behavior of structured surfaces, in particular of superhydrophobic, superamphiphobic and slippery surfaces. We introduced laser scanning confocal microscopy as a novel and extremely powerful tool to explore static and dynamic properties of (multicomponent) liquids on hydrophobic surfaces. We are combining synthesis of model-structures, analysis of microscopic and macroscopic features with complementary experimental techniques and modeling by mean-field descriptions.

High-throughput development of advanced battery materials

Eric McCalla*

Chemistry Department, McGill University, Canada

Abstract:

Advanced battery materials for next-generation technologies involve complex chemistries (at least pseudo-quaternary). These materials all lie in systems where only a handful of compositions have been explored. Furthermore, in cases where further substitutions may prove useful, only a few substituents are typically considered. To fully understand the impact of composition and structure upon the battery properties, thousands of samples are required. Herein, I will present the suite of high-throughput methods (892 samples/week) developed and utilized in my lab to determine both structure and performance of important battery components. These include X-ray diffraction, electrochemistry (to yield important metric such as energy density, cycling stability, and electrochemical stability window), electrochemical impedance spectroscopy (to determine ionic conductivity and stability against metallic anodes), and DC conductivity measurements. These methods, all in high throughput, permit the systematic design of cathodes, anodes and solid electrolytes. This presentation will then focus on 3 systems of note where we have already made important contributions. (1) The entire Li-La-Ti-O phase space for solid electrolytes for Li batteries where metastability plays an important role improving conductivities. (2) The Na-Fe-Mn-O system for cathodes for Na-ion batteries where performance optimization has yielded state-of-the- materials with improved air stability. (3) Finally, we recently applied HTS to increase the ionic conductivity of Na-Zn-Si-O/ionic liquid hybrid electrolytes by a factor of 40 to reach 0.6 mS/cm at room

temperature with a large electrochemical stability window. These 3 studies, involving over 1000 compositions, have resulted in better materials and advanced our understanding of the underlying materials science.

Biography:

Eric McCalla completed his PhD at Dalhousie in 2013 and a post-doc at the Collège de France in 2015, both in battery materials research. Following this, he completed a post-doc at the University of Minnesota looking at electronic and magnetic properties of complex oxides. Since 2018, he is an assistant professor in the Chemistry department at McGill University.

His group focusses on developing and applying high-throughput methods to accelerate the development of advanced battery materials. He is the co-author of 39 articles (for 7 of these he is the principal investigator).

New Strategies for Magnetic Nanoparticles in Industrial Biotechnology

Sonja Berensmeier[1*]
Paula Fraga Garcia[1]
Sebastian Schwaminger[1]

[1]Technical University of Munich, School of Engineering and Design, Bioseparation Engineering Group, Germany

Abstract

The separation of macromolecules like nucleotides and proteins using magnetic particles has been established on a laboratory scale for many years.

In addition to the very simple separation of particles from complex unclarified fluids, magnetic particles have very high effective specific surfaces (without mass transport limitations), which, depending on their size, can even be much larger than those of classical chromatography materials.

However, in order to make the technology economically competitive on a technical scale, several groups are working on the different particle types, but less on low cost particles and process engineering concepts under high hygienic standard.

In this lecture, current work in the field of technical separation of proteins by magnetic separation is presented and process-related pros and cons are discussed. Since economic processes are unthinkable without low-cost magnetic particles, low-cost iron oxide particles and a new tag system for proteins are presented, which enables highly selective binding between target protein and particle with no need for functionalization of the particles. Depending on tag and surrounding conditions, these interactions can be reversible or irreversible, so that innovative immobilization strategies can be implemented by theses tags.

Biography:

For over 10 years Sonja Berensmeier holds the professorship in Bioseparation Engineering at the Technical University of Munich in Germany, after several years as a group leader at the Karlsruhe Institute of Technology in the area of biofunctional surfaces. She meets the challenge for applied integration of molecular biology, biotechnology, particle technology, and process engineering. The focus of the current research is process development of new adsorptive and extractive separation methods. In the field of adsorbents she is specialized in magnetic and conductive particles and the development of new suitable process concepts.

Advanced Nanostructured Materials for the Selective Detection of Gaseous Compounds

Andrea Gaiardo

MNF-Micro Nano Facility, Sensors and Devices Center, Bruno Kessler Foundation, Via Sommarive 18, Trento, 38123, Italy

Abstract

Nowadays, the development of innovative and low-cost smart gas sensors is pursued for many applications, including environmental monitoring, medical screening and precision farming. Chemoresistive gas sensors are the most widely studied solid state gas sensors in this perspective, due to their high sensitivity, small size and low production cost. However, the lack of selectivity and long-term stability of the most widely used class of sensing material so far, i.e. nanostructured metal oxides (MOX), limited the effective and widespread adoption of these devices in many applications. In order to overcome these shortcoming, great attention has been paid on the development of innovative sensing materials with advanced chemoresistive properties in the last few years, seeking the optimization of the sensing performance. Metal sulphides, functionalized/modified MOX, organic-based nanomaterials, metal organic frameworks and new 2D compounds (e.g. phosphorene) are just a few examples of the wide palette of innovative materials studied, which revealed both positive and negative aspects in gas detection. Although none of them represented a definitive solution to the search for the optimal active material for gas sensing, they proved to be extremely useful in meeting specific requirements for individual applications. In this presentation, an overview on micro and nanotechnologies developed at the Bruno Kessler Foundation (FBK) towards the improvement the gas sensor performance and the optimization of sensor production process will be presented. In particular, there will be a focus on the latest results obtained with innovative nanostructured materials for gas detection.

Biography:

Andrea Gaiardo received the Ph.D. degree in Physics from the University of Ferrara in 2018. Currently, he is a researcher in the Micro-Nano Facilities group of the Bruno Kessler Foundation. His work is focused on the research and development of gas sensing systems for several applications, including precision agriculture and outdoor air quality monitoring. He has collaborated in both national and European projects, funded by either private or public entities. He is also a co-founder of the start-up SCENT s.r.l., which develops gas sensing systems for the screening of colorectal cancer.

Cellulose Derivatives and Nanocrystals and Their Liquid Crystalline Properties: Exploitation for Engineering Materials

Susete N. Fernandes[1*]
P. Grey[1,2]
D. V. Saraiva[1]
R. Chagas[1]
Pedro L. Almeida[1,3]
P.E.S. Silva[1]
Luís Pereira[1,2]
Maria H. Godinho[1]

[1]i3N/CENIMAT, Department of Materials Science, NOVA School of Science and Technology, NOVA University Lisbon, Campus de Caparica,Caparica, Portugal

[2]CEMOP/UNINOVA, Campus de Caparica, 2829-516 Caparica, Portugal

[3]Physics Department, ISEL, R. Conselheiro Emídio Navarro, 1, 1959-007 Lisboa, Portugal

Abstract

Cellulose can be found in plants in the form of a bundle of nanofibrils, where elongated crystalline domains are parted from disordered regions. If one removes the disordered regions, cellulose nanocrystals (CNCs) are obtained. In the form of a stable aqueous suspension, CNCs self-assemble into a liquid crystalline (LC) phase giving rise to solid structures with tunable structural coloration1,2. The chemical versatility of cellulose also leads to a well-known variety of derivatives that can present LC phases. This feature that also impart distinct and interesting properties to the final product but is less exploited in producing new materials. In this small overview, the use of CNCs and cellulose derivatives, derived from the LC phase, on the development of innovative and/or biomimetic materials are shown. For example, all-cellulosic composite systems of hydroxipropylcellulose/CNCs can generate biomimetic diffraction gratings with anisotropic mechanical properties3; if an inversion of host/guest is done, structures that reflect NIR wavelength are obtained4. Furthermore, multi-photoresponsive surfaces with opposite wettability can be made from acetoxypropylcellulose LC phases5. Micrometric CNCs films, produced from the LC phase, can be used as solid electrolyte on field-effect transistors to generate circularly polarized light (CPL) sensors6. If microgaps, found within the cross-section of CNCs films, are infiltrated with a nematic liquid crystal, a tunable left- and right-handed CPL system is achieved7. LC phase of hydroxypropylmethylcellulose displays traveling colored patterns with change in the sign of the helix pitch8. These examples open new horizons for the application of these renewable materials.

Biography:

1- Almeida et al. Adv Mat, 30, 1703655, 2018; 2- Fernandes et al. Curr Opin Solid State Mater Sci, 23, 63, 2019; 3- Fernandes et al. Macromol Chem Phys, 214, 25, 2013; 4- Saraiva et al. Crystals, 10, 122, 2020; 5- Fernandes et al. 23, 465, Cellulose, 2016; 6- Grey et al., Adv Funct Mater, 29, 1805279, 2019; 7- Fernandes et al. Adv Mat, 29, 1603560, 2017; 8- Silva et al. Commun. Mater. 2, 79, 2021.

Creep of EN-AW 2024 Aluminum Alloy: Experiment and Damage Evolution Model

Adam Tomczyk[1*]
Andrzej Seweryn[2]

[1]Białystok University of Technology, Poland

[2]Gdańsk University of Technology, Poland

Abstract

The presented research relate to short-term creep-rupture tests of samples made of the 2024 alloy in the T3511 temper under uniaxial tensile stress conditions. Tensile tests carried out at room (20°C) and elevated (100°C, 200°C, 300°C) temperatures made it possible to determine strength properties of the material (Young's modulus, yield stress, ultimate tensile strength) [1, 2] and parameters K and n of the Ramberg–Osgood equation [3]. Creep tests were performed for several different levels of nominal axial stress (load) at each temperature according to the ISO standard [4]. It was observed that in the process of creep to failure at 200°C and 300°C, as the stress decreases, the creep time increases and, at the same time, the strain at rupture increases. However, such a regularity is maintained until a certain transition stress value σt is reached. Reducing the stress below this value results in a decreased value of the strain at rupture. A microscopic analysis of fractures was also performed, thanks to which the mechanisms of material damage and fracture were identified.

The results of the investigation were used to develop a simple, two-parameter model of damage accumulation for the stress range above the transient value [3]. The increase in the isotropic damage state variable was made dependent on the value of axial stress and the increase in plastic axial strain. Using the results of experimental creep-rupture tests and the failure condition, the parameters of the proposed model were determined.

Biography:

[1] Tomczyk A., Seweryn A., Grądzka-Dahlke M. (2018), The effect of dynamic recrystallization on monotonic and cyclic behaviour of Al-Cu-Mg alloy, Materials, Vol. 11, p. 874.
[2] Tomczyk A., Seweryn A., Doroszko M. (2018), Monotonic behaviour of typical Al-Cu-Mg alloy pre-strained at elevated temperature, Journal of Theoretical and Applied Mechanics, Vol. 56, pp. 1055-1068.
[3] Tomczyk A., Seweryn A. (2021), Experimental investigation and modeling of damage accumulation of EN-AW 2024 aluminum alloy under creep condition at elevated temperature, Materials, Vol. 14, p. 404.
[4] EN ISO 204: 2009, Metallic Materials, Uniaxial Creep Testing in Tension: Method of Test; ISO: Geneva, Switzerland, 2009.

A Quantum-Mechanical Study of Anomalous Magneto-Volumetric Behavior of Ferromagnetic Ni31Mn25Sn8 Alloy

M. Friák[1*]
M. Mazalová[1,2]
I. Turek1
O. Schneeweiss[1]
J. Kaštil[3]
J. Kamarád[3]
M. Šob[2,1]

[1]Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, 616 00 Czech Rep.

[2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, 611 37, Czech Rep.

[3]Institute of Physics, v.v.i., Czech Academy of Sciences, Prague 8, 182 21 Czech Rep.

Abstract

We have performed an ab initio study of disordered ferrimagnetic Ni31Mn25Sn8 martensite. Employing the supercell approach combined with the special quasi-random structure concept for modeling of disordered states we have determined thermodynamic, magnetic, structural, elastic and vibrational properties of the studied material. Its atomic and magnetic configuration is found to exhibit a pressure-induced increase of the total magnetic moment, i.e. the total magnetic moment increases with decreasing volume. This highly anomalous trend in the total magnetic moment is revealed despite of the fact that the magnitudes of local magnetic moments of atoms decrease with decreasing volume (as is common in magnetic systems). The origin of the identified phenomena may be related to (i) the ferrimagnetic nature of the magnetic state when the parallel and antiparallel magnetic moments nearly compensate each other and (ii) chemical disorder that leads to different local atomic environments and, consequently, also to different local magnetic moments and their different response to hydrostatic pressures (the antiparalell moments are more sensitive to pressures). The studied state is mechanically and dynamically stable (no imaginary-frequency phonons) but, regarding its thermodynamic stability, it is an excited state (see M. Friák et al., Mater. Trans. (2022) in press, doi:10.2320/matertrans.MT-MA2022006).

Biography:

Martin Friák works as a group leader at the IPM in Brno (CZ). He is a theorist performing quantum-mechanical calculations of materials. After PhD studies of solid state physics at Masaryk University in Brno, he spent 11 years in Germany: first as a post-doc in the Theory department of Prof. Matthias Scheffler at the Fritz Haber Institute of the Max Planck Society in Berlin (2002- 2005) and then as a group leader in the Computational Materials Design department of Prof. Jörg Neugebauer at the Max Planck Institute for Iron Research in Dűsseldorf (2005-2013). Over 100 publications, 3500 citations, H-index 29.

Materials Informatics of High Entropy Alloys

Stefanos Papanikolaou*

NOMATEN, NCBJ, Poland

Abstract

Predicting features of mechanical deformation represents a fantastic challenge as it depends

on a myriad of factors related to material microstructure, specimen geometry and loading conditions. Micromechanical approaches try to bridge microstructural features of solids with their mechanical response, but they are confronted to the high level of complexity of microstructures and microscopic damage processes involved in materials, especially in multicomponent crystalline materials, such as high entropy alloys. Recently, new approaches inspired from data science have emerged: the key microscale parameters that control mechanical deformation at large scale can be identified, and even learned, from the statistical analysis of a large amount of data. Statistical predictions range in a wide gamut of applications, from indentation of composites, to neural networks for understanding of elastic and plastic features of deformation in crystals. I will present a set of tools that utilize the dynamical stability of elasticity as an asset towards microstructural characterization and parameter-free multiscale modeling. Through this approach, I will demonstrate applications for synthetic data and will discuss possible experimental validation routes.

Biography:

Stefanos Papanikolaou acts as a Research Group Leader of the Materials Structure, Informatics and Function (MASIF) Group, in the NOMATEN Center of Excellence for Multifunctional Materials in the National Center for Nuclear Research in Poland. His BSc is in Physics from the National University of Athens. His MS and PhD degrees are in Physics from the University of Illinois, Urbana-Champaign. He performed his postdoctoral work in the Department of Physics at Cornell University, and then he held positions at Yale University, Johns Hopkins University and West Virginia University. Papanikolaou won the internationally competitive 5-year VIDI excellence grant by the Netherlands research council in 2013 and a research excellence award in 2018. His research interest is in the theories and applications of statistical methods for the multiscale modeling of mechanical behavior of materials, as well as their connection to material informatics and machine learning methods.

Clusters of Bio-Synthetic Compartments as Novel Nanotheranostics

Cornelia G. Palivan[1,2*]

[1]University of Basel, Chemistry Department, Mattenstr. 24a, 4002 Basel, Switzerland

[2]University of Basel, Swiss Nanoscience Institute, Mattenstr. 24a, 4002 Basel, Switzerland

Abstract:

Here we present how DNA-directed arrangement of soft synthetic nanocompartments serves to generate super-assemblies with emergent properties, which can be loaded with biomolecules and/or imaging agents in order to develop medical applications. The size and stability of the resulting DNA-linked compartment clusters have been controlled by manipulating molecular factors such as compartment membrane composition and DNA surface density. These clusters can interact selectively with different cell lines, opening a new strategy to modify and expand cellular functions by attaching them on cell surfaces. To display the breadth of therapeutic applications attainable with our system, we encapsulated medically established enzymes within the inner compartment and demonstrated their activity within the clustered compartments. A step forward has been achieved when such DNA-zipped compartments were able to serve as segregated nanospaces containing therapeutic enzymes (Dopa decarboxylase, DDC) and fluorescent probes for development of nanotheranostics. The diagnostic compartment provides a twofold function: tractability via dye-loading as the

imaging component and the ability to attach the cluster construct to the surface of cells. The therapeutic compartment, loaded with active DDC, triggers the cellular expression of a secreted reporter enzyme via production of dopamine implicated in atherosclerosis. Such DNA-zipped clusters of nanocompartments equipped with biomolecules can be expanded by diversifying the types of utilizable active molecules and thus expand the breadth of attainable applications.

Biography:

Cornelia Palivan is currently Professor of Physical Chemistry in the Chemistry Department at the University of Basel. The main focus of her research group is at the interface between physical-chemistry, nanoscience and biophysics, with particular emphasis on bio-nano-systems for translational applications. Her research interests are in the field of developing hybrid functional materials based on combinations of biomolecules with synthetic assemblies, and their interactions with cells or microorganisms. She published more than 170 research articles and reviews in the field, and received various prizes. She is international expert for evaluation of research projects (e.g. ERA-Chemistry and ERC grants program EU).

Current and Future of Red and Black Phosphorus Nanomaterials

Hai-Feng Ji*

Department of Chemistry, Drexel University, Philadelphia PA 19104

Abstract

I will present a summary of some optoelectronic applications of red and black phosphorus nanomaterials. The synthesis, characterization, stability improvement of the materials will also be discussed.

Biography:

Hai-Feng (Frank) Ji is current a professor of Department of Chemistry, Drexel university. His research interests focus on MEMS devices, nanomaterials for energy and environmental applications, drug discovery, nanopillars and phosphene for energy applications, and surface chemistry. He is currently a co-author of 200 peer-viewed journal articles and book chapters. He has an H-index of 40. He is an editorial board member of several chemistry journals.

Micromagnetic Techniques for Steel Characterization

Thomas W. Krause[1*]
Mehrdad Kashefi[1]
P. Ross Underhill[1]
Aroba Saleem[1]
Shannon P. Farrell[2]

[1]Department of Physics and Space Science, Royal Military College of Canada, Kingston, ON, K7K 7B4, Canada

[2] Defence Research and Development Canada, Atlantic Research Centre, Dartmouth, NS, Canada

Abstract

Ferromagnetic steel product is pervasive in our society, with vital applications arising in

electrical steels, oil and gas pipelines, naval structures, aircraft landing gear and automotive components. This presentation communicates recent progress in the characterization of steel materials using the micromagnetic technique, magnetic Barkhausen noise (MBN). Effects on MBN due to changes in microstructure, such as migration of impurity elements and modification of precipitate density, and consequent interaction with evolving magnetic domain structure under applied stress and varying magnetizing conditions, are presented. MBN results from abrupt changes in local magnetic domain structure arising under a time-varying magnetic field. In particular, abrupt movement of domain walls occurs as they overcome local pinning barriers. Tempering, which can lead to temper embrittlement, reduces pinning density within grains, as carbides and impurity elements move to grain boundaries, thereby reducing measured MBN. In contrast, presence of elastic stress increases MBN due to refinement of domain structures. These two competing effects complicate identification of degree of embrittlement in the presence of residual stress. Evaluation of MBN energy ratio for magnetization applied parallel and perpendicular to applied tensile stress in Q1N samples revealed that, at the flux density where MBN is almost entirely due to 180° DW motion, the ratio was robustly correlated with applied uniaxial tensile stress level, regardless of degree of tempering, allowing separation of effects of tempering from those of residual stress. Results are explained in light of the anisotropic effect of stress compared with isotropic effect of pinning density on MBN generation.

Biography:

Thomas W. Krause received a B.Sc. degree from University of Calgary, Alberta, Canada, in 1987, and M.Sc. and Ph.D. degrees in Solid State Physics from McMaster University, Hamilton, ON, in 1989 and 1992, respectively. He was with Applied Magnetics Group, Queen's University, Kingston, ON, from 1992 to 1996, after which he took a position with Chalk River Laboratories, ON. In 2006 he moved to Royal Military College of Canada, Kingston and became full Professor in 2008. He has 30 years of research and development experience on non-destructive evaluation technology with a focus on eddy current and magnetic Barkhausen noise.

Characterization of the Performance of Building Components in The Form of PET Fibers Regarding Fire Reaction, Sound Insulation and Conditioning

Maria Fernanda de Oliveira[1*]
Lorenzo Azevedo Kerber[2]
Matheus Donadello[3]
Roberto Christ[4]
Fernanda Pacheco[5]

[1,2,3,4,5]Universidade do Vale do Rio dos Sinos – Unisinos, Brazil

Abstract

The application of polymeric components under the shape of fibers has become usual in acoustic insulation of buildings, being able to meet the performance requirements regarding confort, thermal performance, as well as fire reaction, proposing a sustainable reuse for materials that are largely discarded as domestic residues, such as PET. Therefore, alongside the aspects related to mitigating environmental impacts, these products must be adequately characterized for application, following performance criteria. Often, when selecting construction components, the attendance of fire reaction parameters should be a priority, where laboratory evaluations indicate that the smaller the surface density and thickness of

an element, there will be less burn product, indicating a better fire reaction performance. However, when decreasing these parameters, there is a decrease in the acoustic absorption of these materials. The aim of this work is to present the different performance characteristics of PET lining as of insulation to airborne and impact sound, sound absorption and fire reaction. It is verified that, for the specimens studied, there is an increase in the sound absorption coefficient (about 35%) and airborne and impact sound insulation when there is an increase in the element's surface density. However, it is verified a contrary behavior regarding fire reaction, producing an increase in fire spread, evaluated by the FIGRA parameter, obtained through the SBI test, varying about 89,1 W/s between the two extreme cases.

Biography

Maria Fernanda de Oliveira has a degree in Architecture and Urbanism at Unisinos University, master's in civil engineering at UFSM, Ph.D. in Engineering at UFRGS and postdoctoral in LNEC/ Lisbon. Currently, she works at Unisinos University as coordinator of the Technological Institute in Performance and Civil Construction itt Performance, professor at PPG in Architecture and Urbanism and Editor-in-Chief of ArquiteturaRevista. She is a member of the Brazilian Acoustic Society and has experience in applied research with an emphasis on building acoustics, building performance and material performance.

Characterizing the Tensile Strength of the Fabrics Materials under Radiant Heat Exposure.

Nur-Us-Shafa Mazumder [1]
Sumit Mandal [1*]
Robert J. Agnew [2]
Adriana Petrova [1]
Lynn M. Boorady [1]
Guowen Song [3]

[1]Department of Design, Housing and Merchandising, Oklahoma State University, USA

[2]Fire Protection and Safety Engineering Technology Program, Oklahoma State University, USA

[3]Department of Apparel, Events & Hospitality Management, Iowa State University, USA

Abstract

More than sixty thousand firefighters' injuries have been reported by the National Fire Protection Association (NFPA) in U.S. in 2019. Inadequate protection of the uniform worn by the firefighters could be reason for most of the injuries. Firefighters repeatedly encounter various hazards especially thermal hazards during routine exercise, on-site firefighting, and emergency rescue. Degradation could occur on the bunker gear's fabric, which comes repeatedly in direct contact to thermal hazards when worn in the fire ground. It has also been found that performance of the fabric is extensively affected by the moisture accumulated in the fabric, which may come from the wearers' sweat. Proper evaluation of the tensile strength of the high-performance fabrics used in both single and multi-layer clothing system could help maintain the overall integrity of the uniform. This study focuses on evaluation of tensile strength of the fabrics when exposed to 10, 15, and 20 kW/m2 radiant heat fluxes. Different levels of moisture were added to the test samples to simulate the wearers' sweating. In each fabric system, a total of sixty-four different samples were prepared for four different types of fabric, four levels of moisture and exposed for five minutes. Results show that heat flux and moisture levels have significant impact on fabric tensile strength. Effect of moisture on tensile

strength in three-layered fabric system was higher than the single layer fabric. This study leads to an understanding on the impact of fabric strength in the presence of fire and moisture. Biography: Dr. Sumit Mandal is an Assistant Professor of Textile Science in the Department of Design, Housing and Merchandising (DHM) at Oklahoma State University (OSU), USA. He did his Postdoc from Empa - Swiss Federal Laboratories for Materials Science, Switzerland; PhD from University of Alberta, Canada; Post Graduate Certificate from Nottingham Trent University, United Kingdom; Masters from The Hong Kong Polytechnic University, Hong Kong; and Bachelors from Calcutta University, India. His teaching interests mainly associated with textile science, quality control, and sustainability related courses at OSU. His research primarily focuses on thermal protective textiles, clothing, and equipment for the safety of high-risk sector workers. He is motivated to develop new equipment and protocols for testing the textile materials used in protective clothing under different hazardous exposures such as flame, radiant heat, hot surface, steam, hot water splash, and chemicals. He also supervises graduate students at OSU in the field of protective clothing for different occupational hazards and acts as scientific reviewer and associate editor for many peer reviewed journals (e.g., AATCC Journal of Research, Textile Research Journal, International Journal of Occupational Safety and Ergonomics). He has published 1 book, 8 book chapters, more than 40 journal papers, and presented his research work in different countries such as India, China, Hong Kong, Japan, Croatia, Czech Republic, Switzerland, Greece, Spain, Portugal, Germany, Belgium, England, Canada, and the USA. He has secured funding from various national and international agencies and designated as a Killam Laureate in the field of Natural Science and Engineering from Canada. He is the professional member of the International Textile and Apparel Association (ITAA), American Association for Textile Chemists and Colorists (AATCC), OSU Fire Council, and currently actively contributing for the USA NC 170 Multistate Research Project on Personal Protective Technologies for Current and Emerging Occupational and Environmental Hazards. He is now acting as a Guest Editor in MDPI Polymer Journal for a Special Issue on Recent Advances in Textiles and Fibers.

A Stabilized Mixed P1/P1 Finite Elements with Orthogonal Subgrid Scale for Bingham Flows. A regularized viscoplastic Model

Elvira Moreno[1*]
Miguel Cervera[2]

[1]Watershed Managment Departament, Forestry Engineering School, Los Andes University (ULA), Venezuela

[2]International Center for Numerical Methods in Engineering, CIMNE, Catalonia University (UPC), Spain

Abstract

This present paper deals with the application of a stabilized mixed pressure/velocity finite element formulation for the solution of viscoplastic non-Newtonian flows. Bingham model is considered. This materials exhibit a yield stress, which must be exceeded before deformation can occur. The detail of the discretization procedure is presented, and the Orthogonal Subgrid Scale (OSS) stabilization and the Split Orthogonal Subgrid Scale Stabilization (Split-Oss) techniques are introduced allowing the use of equal order interpolations in a consistent way. The matrix form of the problem is given. A double viscosity regularized Bingham model is introduced as an alternative to the regularized Papanastasiou model. The analytical solution to a Poiseiulle flow has been obtained and a convergence test result is shown to compare both models. Initially, the investigation was centered in the study of viscoplastic flow in cavity, but once the proposal regularized model was introduced, it was applied to viscoplastic flow

with free surface with the objective of studying viscoplastic debris flow. Then, a simplified Eulerian method solved on a fixed mesh is presented to track the movement of the free surface. This is done by transporting the free surface with a stabilized level set method. The numerical solutions are compared with analytical, experimental results and numerical benchmarks from the literature. The extrusion Bingham fluid is presented. The evolution of the streamlines, yielded and unyielded region are shown. The dam break problem results are also compared with field data in the flow due to the failure of a mining reservoir. Keywords: Bingham flows, Split- Orthogonal Subgrid Scale stabilization, viscoplastic regularized model, level set method, free surface, debris flow, extrusion, dam break

Biography:

Elvira Moreno is a researcher in the computational fluid dynamic, specifically, in the field of viscoplastic fluid as in the building seismic design field using the finite elements. She was awared a doctoral fellowship of Los Andes University and granted the Structural Analysis PhD in the Technological University of Catalonia, Spain, in 2014. In 2010, she got the Advanced Studies.

Keynote Session-II

Adventures and Discoveries in Two-Dimensional Ferroelectrics

Sokrates T. Pantelides*

Department of Physics and Astronomy and Department of Electrical and Computer Engineering

Abstract

Ferroelectric materials, analogs of ferromagnets entailing electrical instead of magnetic dipoles, are useful for applications in memories, field-effect transistors, sensors/actuators, etc. Transition-metal oxides have been the primary ferroelectrics, but layered ferroelectrics, bonded by weak van-der-Waals (vdW) interactions and thinned to nanoscale dimensions or even monolayer form, offer significant advantages. The focus of the talk will be on the layered vdW ferroelectric CuInP2S6. This material is also an ionic conductor with the same ions, in this case Cu ions, being responsible for both ferroelectric displacements and ionic conduction. We will describe a synergistic theory-experiment journey that led to a series of discoveries of extraordinary properties1-3: instead of the usual double-well potential for ferroelectric displacements, CuInP2S6 features a quadruple-well potential, corresponding to low- and high-polarization phases, with four polarization states; in addition to regular ferroelectric switching among these four states, an external electric field can also drive the Cu ions across the vdW gaps, signaling a polarization re-alignment against the applied electric field and unveiling a novel mechanism to realize negative capacitance. Finally, we will visit the world of monolayer ferroelectrics with out-of-plane polarization, and describe theoretical predictions of novel monolayer ferroelectrics and heterostructure-based devices4, including a single-atom-thick monolayer antiferroelectric with out-of-plane dipoles5.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences,materials Science and Engineering Directorate.

*Collaborators are the co-authors of the cited papers:

1. J. A. Brehm, S. M. Neumayer, L. Tao, A. O'Hara, M. Chyasnavichus, M. A. Susner, M. A. McGuire, S. V. Kalinin, S. Jesse, P. Ganesh, S. T. Pantelides, P. Maksymovych and N. Balke, "Tunable quadruple-well ferroelectric van der Waals crystals", Nature Mater. 19, 43-48 (2020).

2. S. M. Neumayer, L. Tao, A. O'Hara, J. Brehm, M. Si, P.-Y. Liao, T. Feng, S. V. Kalinin, P. D. Ye, S. T. Pantelides, P. Maksymovych and N. Balke, "Alignment of Polarization against an Electric Field in van der Waals Ferroelectrics", Phys. Rev. Appl. 13, 064063 (2020).

3. S. M. Neumayer, L. Tao, A. O'Hara, M. A. Susner, M. A. McGuire, P. Maksymovych, S. T. Pantelides and N. Balke, "The Concept of Negative Capacitance in Ionically Conductive Van der Waals Ferroelectrics", Adv. Energy Mater. 10, 2001726 (2020).

4. X. Jin, Y.-Y. Zhang, S. T. Pantelides and S. Du, "Integration of graphene and two-dimensional ferroelectrics: properties and related functional devices", Nanosc. Horiz. 5, 1303-1308 (2020).

5. N. G. Richardson, A. O'Hara and S. T. Pantelides, "Out-of-plane antiferroelectricity in a single-atom-thick monolayer", to be published (2021).

Biography:

Sokrates T. Pantelides received a Ph.D. in physics from the University of Illinois at Urbana-Champaign in 1973. He served as Research Staff Member, Manager, Senior Manager, and Program Director at the IBM T. J. Watson Research Center until 1994 when he joined the faculty at Vanderbilt University as the McMinn Professor of Physics. Since 2010, he is also University Distinguished Professor of Physics and Engineering. His research work is theoretical/ computational and spans a wide range of materials, nanostructures and properties. He is the recipient of several awards. He is a Fellow of the American Physical Society, the Materials Research Society, the Institute of Electrical and Electronics Engineers, and the American Association for the Advancement of Science.

Nanotechnology Enabled Metallurgy

Xiaochun Li

Raytheon Chair in Manufacturing, Mechanical and Aerospace Engineering & Materials Science and Engineering, University of California, Los Angeles (UCLA)

Chief Technology Officer, Western Smart Manufacturing Center, DOE Clean Energy Smart Manufacturing Innovation Institute

Abstract

High performance metals offer tremendous potential to improve energy efficiency and system performance for numerous applications. However, conventional processing methods in metals manufacturing have reached certain limits in further improving the properties of metals. Incorporation of nanoelements into various functional materials can obtain unusual physical, chemical, and mechanical properties. This talk will present our latest scientific and technological progress on how nanotechnology can be applied to break metallurgical barriers, enabling unprecedented micro/nano-structure control and property tuning in solidification processing of metals. This nanotechnology enabled metallurgy is poised to create a new age of metals to meet energy and sustainability challenges in today's society.

Biography:

Xiaochun Li is the Raytheon Endowed Chair in Manufacturing Engineering in the Departments of Mechanical and Aerospace Engineering & Materials Science and Engineering at University of California, Los Angeles (UCLA). He currently serves as the Chief Technology Officer for the Western Smart Manufacturing Center, USA Clean Energy Smart Manufacturing Innovation Institute. He received his Ph.D. at Stanford University in 2001. He is a holder of multiple best paper awards and patents, including more than 10 of those licensed by industry. Dr. Li received National Science Foundation CAREER award in 2002, Jiri Tlusty Outstanding Young Manufacturing Engineer Award from Society of Manufacturing Engineers in 2003, and 2008 Howard F. Taylor Award from American Foundry Society (AFS). Dr. Li was previously a professor in the Department of Mechanical Engineering and Materials Science Program at University of Wisconsin-Madison (UW-Madison) from 2001 to 2013. He served as the Director of Nano-Engineered Materials Processing Center (NEMPC) at UW-Madison between 2009 and 2013. Dr. Li has been elected Fellows in National Academy of Inventors, American Society of Mechanical Engineers and the International Society for Nanomanufacturing.

Oral Session-II

Fabrication and Characterization of a Complex Lighting System Formed by a Luminescent Polymeric Rod

R. Narro-García*[1]
E. Olivas-Rodríguez[1]
C.G. Nava-Dino[1]
M.C. Maldonado-Orozco[1]
J.P. Flores-De los Ríos[1]
L. F. Corral-Martínez[2]
F. Espinosa-Magaña[3]
E. Rodríguez[4]

[1]Faculty of Engineering, Autonomous University of Chihuahua, Mexico.

[2]Chihuahua Technological Institute, Division of Postgraduate Studies, Mexico.

[3]Center for Research in Advanced Materials, Mexico.

[4]National Polytechnic Institute CICATA-Unidad Altamira, Mexico.

Abstract

Illumination is one of the most important elements of any room or workspace; it is defined as the deliberate use of light to achieve practical or aesthetic effects. The latter, has inspired the design of complex lighting systems such as fibre optic Christmas trees or photoluminescent optical fibres with lateral emission in which the light color is a combination of the light source and the photoluminescence of the active material. Since the intended use of most of these complex lighting systems are mainly decorative, there is a lack of information regarding its performance or manufacturing process. The complex lighting systems proposed is formed by a poly (methylmethacrylate) (PMMA) rod covered by a polymer thin film that contains luminescent nanoparticles. A spray process was used to deposit the thin film with different luminescent particles concentration. The structure, morphology and optical properties of the samples were measured by X-ray diffraction, atomic force microscopy, UV-VIS and photoluminescence spectroscopy, respectively. Results showed that polymer based

composite luminescent material could be a good candidate for the development of complex lighting systems.

Biography:

Roberto Narro García was born in Tampico, Mexico in 1981. He received his Doctorate degree in Advanced Technology from the National Polytechnic Institute in 2012. In the same year he joined the Center for Research in Optics as a post-doctoral researcher where he continued working with soft glasses and luminescent nanoparticles for two years. After that, he started a new postdoctoral project at the Center for Applied Physics and Advanced Technology focused on polymer optical fibers. Since 2016 he has working as an Academic at the Faculty of Engineering of the University Autonomous of Chihuahua.

Novel 2D MXene Based Nanocomposites for Disease Early Detection and Prevention

Danling Wang[*1,2]
Sampada Koirala[2]
Anna Rudie[1]
Qifeng Zhang[1,2]

[1]Depart. Electrical and Computer Engineering, North Dakota State University, Fargo, USA

[2]Biomedical Engineering Program, North Dakota State University, Fargo, USA

Abstract

Acetone existing in human breath is an effective biomarker of diabetes, which can be used for the early diagnosis and daily monitoring of diabetes. Comparing to the conventional method of monitoring the blood glucose level in blood, detection of breath acetone provides a non-invasive, accurate, convenient, and inexpensive method of diabetes diagnosis and monitoring. In this presentation, we report a new breath acetone sensor based on a novel 2D MXene based nanocomposite made by 1-dimensional nanorods, K2W7O22 (KWO) and 2-dimensional Ti3C2 MXene. The results indicated that the lowest detection limit of this sensor for breath acetone can be down to 0.2 parts-per-million (ppm) which is much less than 0.76 ppm, the key threshold to distinguish health person and high-risk of diabetes person. More importantly, the 1D/2D KWO/Ti3C2 nanocomposite based sensor shows excellent selectivity to acetone, great tolerance to water vapor, and can operate at room temperature. This success of this research offers a new sensing technology for disease early detection and health monitoring noninvasively.

Biography:

Danling Wang is an Assistant Professor of the Department of Electrical and Computer Engineering at North Dakota State University. She earned dual Ph.D. in Electrical Engineering from University of Washington and Optical Physics from Peking University. As the principle investigator of NEWS (Nano-Electronic Wearable Sensors) lab, her research focuses on investigation of nanomaterial based sensor devices for applications in industry, military, and breath analysis for early stage disease diagnosis. Since 2016, Dr. Wang and her team have published more than 28 peer-reviewed journal papers and invited conference presentation. Her research has been founded from the NASA, Sanford health, ND EPSCoR grants and NDSU Foundation Awards.

Superconducting Super-Magnets and its Importance for the SDG's

Muralidhar Miryala

Materials for Energy and Environmental Laboratory, College of Engineering / Graduate School of Engineering and Science, SIT, 3-7-5 Toyosu, Koto City, Tokyo 135-8548, Japan.

Abstract

The economic growth and future sustainable development of global community require use of new materials improving quality of life. Superconductivity in general allows for 100% current transmission without losses. This makes it super valuable resource for sustainability in many aspects. The high-temperature superconducting materials (HTSC), which will be crucial for the day-life applications, need to become more attractive for the sustainable development goals (SDG's). In the current era, medical field applications possess the highest priority. With increase in demand for MRI scans, it is necessary to produce high performance magnets cost effectively. The present MRI machines are operated at 4 K, being cooled by liquid helium, while with superconductors such as MgB2 can be operated at 20 K with the help of much economical cooling with cryogen-free refrigerators. The same applies to NMR. In the case of magnetic drug delivery (MDD), we need a sharp and strong magnetic field, which can be delivered by MgB2 bulk. However, the values of the critical current density and the flux pinning force need a considerable improvement, especially at elevated application temperatures like 20-30 K. During this presentation, we will present on optimization of fabrication parameters combined with silver addition, use of nano boron, use of carbon-encapsulated boron (CCB), combined Mg excess and CCB, CCB with Dy2O3 etc. for producing high quality bulk MgB2. In addition, nano-boron precursors were synthesized by ultra-sound to improve the performance and reduce the cost. Eventually, we will report the high trapped field and large critical current values around 20K.

Biography:

Muralidhar Miryala is Board of Councilor at Shibaura Institute of Technology (SIT), Japan, and professor at the Graduate School of Science and Engineering, and College of Engineering, SIT. His main task is to transform SIT into a high rank university. To accomplish this goal, he has been working towards designing numerous innovative programs to enhance global initiatives for SIT. He has published over 500 research items including patents, books, review-articles, articles etc., and delivered over 150 oral presentations, including plenary and invited ones. He has received several awards for his research contributions, including the prestigious 2021 Pravasi Bharatiya Samman Award by the President of India.

Microstructure Evolution of CoNiCrAlY and NiCoCrAlY Alloy by High Temperature Deformation

Makoto Hasegawa*
Maiko Iwashita
Yuji Kubota

Yokohama National University, Japan

Abstract

CoNiCrAlY and NiCoCrAlY alloy has been used as an alloy to protect Ni-base superalloy from oxidation. In the classification based on entropy, those alloys are positioned as a high entropy

alloy. There are reports that high entropy alloys are excellent in environmental resistance as well as mechanical properties. For both alloys which are excellent in environment resistance and can be classified as high entropy alloys, there is a possibility that they may exhibit excellent mechanical properties as well. However, there are few such reports. Furthermore, the possibility of microstructure control in the alloys is still open question. In this study, high temperature compressive deformation was performed on CoNiCrAlY and NiCoCrAlY alloy, and deformation behavior, microstructure and texture formation were experimentally investigated. Uniaxial compression tests were performed from 1073 K – 1473 K and ε̇= 5 x 10-2s-1 – 1 x 10-4s-1. After the test up to e= -1.0, the specimens were cooled immediately by blowing N2 gas. Microstructure observation and EBSD analysis were performed at the cross-section of the specimens. CoNiCrAlY and NiCoCrAlY alloys were composed of (g+b) two-phase and (g'+b) two-phase, respectively. True stress – true strain curves show so-called work softening type indicating occurrence of dynamic recrystallization. Weak textures were observed in g and b phased grains in the CoNiCrAlY alloy and g' phased grains through all Zener-Hollomon parameter (Z) deformation conditions. In case of b phased grains in NiCoCrAlY alloy, texture developed with the decrease in Z value due to change of DRX from nucleation and growth mechanism to bulging mechanism.

Biography:

Makoto Hasegawa obtained Doctor of Engineering (2002) from Yokohama National University, Japan. He worked as a postdoctoral research fellow and research associate in The University of Tokyo from 2002 to 2006 and as a research associate in Yokohama National University from 2006 to 2010. He became an associate professor in 2011, and from 2021, he became a professor in Yokohama National University. His is currently focused on the researches of the high temperature processing on intermetallic and alloys for preferential orientation control, and an orientation control of metals and ceramics coatings produced by aerosol deposition.

An Investigation of Dislocation Density and Work Strengthening in CoCrFeMnNi High Entropy Alloy

Pramote Thirathipviwata*
Yusuke Onukia
Junhee Hanb, Shigeo Satoe

[a]Frontier Research Center for Applied Atomic Sciences, Ibaraki University, Tokai, Ibaraki 319-1106, Japan

[b]Korea Institute for Rare Metals, Korea Institute of Industrial Technology (KITECH), Incheon 21999, Republic of Korea

[c]Graduate School of Science and Engineering, Ibaraki University, 4-12-1 Nakanarusawa, Hitachi, Ibaraki 316-8511, Japan

Abstract

High entropy alloys (HEAs) are designed based on the concept of entropic stabilization associated with a large number of constituent elements (≥ 5) in equiatomic or near-equiatomic ratio. Due to compositional complexity of HEAs, it is expected to perform unique microstructural mechanisms and excellent properties, especially mechanical properties. In CoCrFeMnNi HEA or so-called Cantor alloy, yield strength is largely enhanced by plastic deformation from 222 MPa of homogenized sample to 867 MPa of 85% area reduction sample. In comparison with binary FeNi alloy, the dislocation accumulation of the CoCrFeMnNi HEA

during plastic deformation is significantly larger. The dislocation density was evaluated by neutron line profile analysis with using convolution multiple whole profile (CMWP) method. With the CMWP method, the extensive dislocation arrangement was evaluated in the CoCrFeMnNi HEA. The high compositional complexity, extensive dislocation arrangement and deformation mechanism (i.e., grain fragmentation and deformation twining) facilitates the large dislocation accumulation. The large work strengthening in the CoCrFeMnNi HEA is correlated with large dislocation density during plastic deformation.

Biography:

Pramote Thirathipviwat is a researcher at Frontier Research Center for Applied Atomic Sciences, Ibaraki University, Japan. P. Thirathipviwat completed his Doctor of Engineering at TU Dresden, Germany. His research focuses on metallic alloys (i.e., high entropy alloys), microstructural characterization, and neutron and X-ray diffraction.

Design of Interactive Metahologram via Liquid Crystallinity

Young-Ki Kim*
Won-Sik Kim
Jingang Choi
Yena Choi
Jun Hyung Im

Pohang University of Science and Technology (POSTECH), Republic of Korea

Abstract

The arrays of subwavelength-scaled nanostructures on a surface, often called metasurfaces, have made advances in flat optics because of their potential to display programmable hologram and miniaturize optical components. Because previous metasurface systems are passive, however, their practical applications have been impeded. Accordingly, recent efforts have focused on the realization of active metasurfaces that can switch holograms upon triggers via using, for example, phase-change materials, mechanical actuations, and chemical reactions. Nevertheless, the full potential of active metasurface system has yet to be realized due to the limitation of previous approaches, including limited design of nanostructures, complex fabrication process, and slow response.

Here, we propose a simple and versatile design rule to enable dynamically tunable metahologram systems by leveraging the optical anisotropic and stimuli-responsive nature of liquid crystals (LCs). We demonstrate the new class of active metahologram, a thin layer of LC integrated with multiplexing metasurface, to autonomously sense a programmed stimulus (e.g., electric field, temperature, pressure, toxic gas) and dynamically switch the holographic images [1,2,3]. These attribute provides insight into the rational design of interactive meta-hologram display that enable their full potential of multifunctional active devices. This work was supported by the Korea National Research Foundation (NRF-2021R1A4A1030944 & 2021R1A2C2095010).

[1] "Liquid Crystal Powered Mie Resonators for Electrically Tunable Photorealistic Color Gradients and Dark Blacks", Light: Science & Applications, Accepted (2022)

[2] Science Advances, 7, abe9943 (2021).

[3] Advanced Materials, 32, 2004664 (2020).

Biography:

Young-Ki Kim is currently an Assistant Professor in the Department of Chemical Engineering at POSTECH, Republic of Korea. He received his PhD (2015) in Chemical Physics from Liquid Crystal Institute at Kent State University under the supervision of Prof. Oleg D. Lavrentovich. He then worked as a postdoctoral associate in the laboratory of Prof. Nicholas L. Abbott at University of Wisconsin-Madison (2015–2018) and Cornell University (2018–2019). His research focuses on the design of functional materials using liquid crystallinity. Dr. Kim has published 45 papers in peer-reviewed journal including Nature and Science.

Optimizing the Required Cathodic Protection Current for Pre-Buried Pipelines Using Electrochemical Acceleration Methods

Nguyen Thuy Chung[1]
Min-Sung Hong[1]
Jung-Gu Kim[1*]

[1]School of Advance Materials Engineering, Sungkyunkwan University, 300 Chunchun-Dong, Jangan-Gu, Suwon 440-746, Korea;

Abstract

Several corrosion mitigation methods are generally applied to pipelines exposed to corrosive environments. However, in the case of pre-buried pipelines, the only option for corrosion inhibition is cathodic protection (CP). To apply CP, the required current should be defined even though the pipeline is covered with various oxide layers. In this study, an electrochemical acceleration test was used to investigate the synthetic soil corrosion of a pre-buried pipeline. Potentiodynamic polarization experiments were first conducted to ascertain the corrosion current density in the environment, and galvanostatic measurements were performed to accelerate corrosion according to the operating time. In addition, corrosion current density and the properties of the rust layer were investigated via potentiodynamic polarization tests and electrochemical impedance spectroscopy (EIS) tests. The variation in surface corrosion was subsequently analyzed via optical microscopy (OM) and X-ray diffraction (XRD) measurements. Finally, an empirical equation for the optimized CP current requirement, according to the pipeline service time, was derived. This equation can be applied to any corroded pipeline.

Porous Polymer Films for Absorbing Toxic Dyes Composed of Polypyrrole and Graphene

Do Sung Huh*
Shahkar

Department of Chemistry and Nano Science and Engineering, Center for Nano Manufacturing, Inje University, Gimhae, Gyeongsangnam-do 50834, South Korea

Abstract

In the present study, a honeycomb-patterned (HCP) porous film composed of polypyrrole (PPy), and graphene oxide (GO) was fabricated using modified breath figure method in a single step. For the modified BF method, ferric chloride was included as the oxidant in the

polycaprolactone (PCL) polymer solution and pyrrole (Py) was contained in the water solution for the humidity. The polymerization of Py then takes place at the oxidant vapour interface resulting in pore-selective PPy functionalization. Whereas, GO was included in the PCL polymer solution, present on the interpore surface. The surface morphology of the PPy-GO film was characterized by scanning electron microscopy (SEM). The functionalization of PPy-GO was confirmed by UV–visible spectroscopy, FT-IR, and contact angle measurement. The fabricated porous films were then systemically investigated for the removal of two anionic dyes Congo Red (CR) and Eriochrome Black T (EBT) in aqueous solution. The SEM images together with UV and FT-IR spectra confirmed the functionalization of PPy and GO. Our study demonstrated that PPy-GO porous film is a very promising adsorbent for wastewater treatment.

Keywords: Honeycomb-patterned porous film, polypyrrole, graphene oxide, dye adsorption

Biography:

1984-1986: M.Sc: Department of Chemistry of Korea Advanced Institute of Science and Technology S. Korea

1986-1989: Ph.D: Department of Chemistry of Korea Advanced Institute of Science and Technology S. Korea

1989-present: Professor of Inje University

Toward High-Performance Single-Crystal Perovskite Solar Cells

Fang-Chung Chen1,2*
Hao-Yeu Tsai1
Yung-Fang Yang1
Hong-Sheng Jiang1
0.Chien-Chen Kuo1

[1]Department of Photonics, National Yang Ming Chiao Tung University, Taiwan

[2]Center for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, Taiwan

Abstract

Most perovskite solar cells (PeSCs) are prepared using solution processes and the resulting films are polycrystalline in nature. Defects on the grain boundaries inevitably impede the charge transport, thereby limiting the efficiency of the devices. PeSCs prepared with perovskite single crystals would, in theory, exhibit even higher efficiencies, due to lower trap densities and superior charge transport. Therefore, in this presentation, we will present our recent results in the high-performance single-crystal perovskite solar cells. We develop new a promising but general method, differential space-limited crystallization (DSLC), for synthesizing high-quality perovskite single-crystal micro-plates. The DSLC method does not require very thin spacers, it simplifies the procedure of crystal growth. We also prepared single-crystal PeSCs featuring modified hole-transport layers (HTLs) that improved the power conversion efficiency (PCE). Further, in additional to conventional three-dimensional perovskite materials, we also developed two-dimensional (2D) PeSCs. The insulating chains of the ammonium cations in 2D perovskites inevitably impede charge transport in PeSCs, thereby limiting the power PCEs. Therefore, we also proposed a new space-limited crystallization method for growing asymmetric 2D perovskite single crystals with vertically oriented Ruddlesden-Popper phases. The high crystallinity and preferred orientation of the 2D layered structures reduce the impact

of the bulky side chains of the ammonium cations and facilitate the charge transport in the perovskite SCs. The device performance will be discussed in detail in this talk.

Biography:

Fang-Chung Chen is current a Professor and Chairman of Department of Photonics, National Yang Ming Chiao Tung University. Prof. Chen is a Fellow of the Royal Society of Chemistry (FRSC). He is the recipient of the Award for Junior Research Investigators of Academia Sinica 2008. He is the section editor (Organic Materials) of Encyclopedia of Modern Optics, edition II, Elsevier and a member of Editorial Board for Processes (MDPI) and Current Smart Materials. His h-index is 46 (Google Scholar). His research interests include flexible solar cells, organic/perovskite materials and electronics and low-dimensional nanomaterials.

Low Driving Voltage and High Efficiency Phosphorescent OLED Achieved by New Host Comprising of Acridine-Carbazole-Benzimidazole Moieties

Bo-Yen Lin[1*]
Chia-Hsun Chen[2,3]
Ching-Huang Chiu[2]
Man-kit Leung[3]
Tien-Lung Chiu[1]
Jiun-Haw Lee[2]

[1]Department of Electrical Engineering, Yuan Ze University, Chungli, Taoyuan 32003, Taiwan

[2]Graduate Institute of Photonics and Optoelectronics and Department of Electrical Engineering National Taiwan University, Taipei 10617, Taiwan

[3]Department of Chemistry, National Taiwan University, Taipei 10617, Taiwan

Abstract

Organic light emitting diodes (OLEDs) have attracted great attentions since their unique advantages such as light weight, fast response and flexible application etc., and hence numerous researching efforts had been paid on their progresses on materials, device architecture, fabrication method in past three decades. Among those technologies, thanks to the development of phosphorescent emitters, which result in a great breakthrough in efficiency, that 100% in internal quantum efficiency (IQE) and >30% in external quantum efficiency (EQE) can be achieved simultaneously in phosphorescent OLEDs.

Here, a new host material was successfully synthesized and which exhibited comprised of carbazoles and acridine (Ac) as hybrid electron donor units as well as one benzimidazole as electron acceptor unit, where Ac capable of strong electron donating was employed to lift up highest occupied molecular orbital (HOMO) level to facilitate hole injection and transport in OLED. For photophysical properties, this host exhibited a bandgap of 3.07 eV and also a high triplet energy of 2.99 eV; Such photophysical properties are considered as a suitable host for blue phosphor Bis[2-(4,6-difluorophenyl)pyridinato C2,N](picolinato)iridium(III) (FIrpic). As a results, blue phosphorescent OLED employing this host consequently showed a low turn on voltage of 2.8 V, and high power efficiency in terms of 63.2 lm/W. In addition, current efficiency, external quantum efficiency and color coordinates of this OLED were 60.2 cd/A, 27.7% and (0.16, 0.39), respectively.

Biography:

Bo-Yen Lin received his B.S. degree (2010) in Department of Electronic and Computer Engineering at National Taiwan University of Science and Technology and his M.S. (2012) and Ph.D degree (2017) in the Graduate Institute of Photonics and Optoelectronics in National Taiwan University. After that, he joined Nichem Fine technology Co. Ltd., as a section manager (2017). At present, Dr. Lin work as postdoctoral research in Department of Electrical Engineering at Yuan-Ze University since 2019. His research directions are in OLED and QD-LED which include light management, degradation mechanism and charge and exciton dynamics.

End of Day 4 Parallel Session I

Oral Presentations

Fumaric Acid Incorporated Ag/agar-agar Hybrid Hydrogel: A Multifunctional Avenue to Tackle Wound Healing

Somnath Ghosh[1*]
Sayed Ilias Basha[2]

[1]Indian Institute of Petroleum & Energy, Visakhapatnam, Indian
[2]GITAM Institute of Medical Science and Research, Visakhapatnam, India

Abstract

Wound and its treatment is one of the major health concerns throughout the globe. Various extrinsic and intrinsic factors can influence the dynamics of healing. One such extrinsic factor is moist environment. The advantages of optimum hydration in healing are enhanced autolytic debridement, angiogenesis and accelerated cell proliferation and collagen formation. But hydrated wounds often end up with patient's un-comfortability, associated infection, and tissue lipid peroxidation.

Here, we have synthesized fumaric acid incorporated agar-silver hydrogel (AA-Ag-FA); characterized by UV–Visible spectroscopy, FTIR spectroscopy and TEM. The size of the silver nanoparticles (Ag NPs) was found to be 10–15 nm. The hydrogel shows potential antibacterial effect against Escherichia coli, Staphylococcus aureus and Pseudomonas aeruginosa predominantly responsible for wound infection. The gel shows reasonable antioxidant property evaluated through 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. Topical application of the gel heals the wound at much faster rate even compared to standard (Mega heal, Composition: Colloidal silver 32 ppm hydrogel) gel. Histological analysis reveals better tissue proliferation (i.e. epithelialization), more granulation tissue formation, neovascularisation, fibroblast and mature collagen bundles. The lipid peroxidation of wound tissue estimated through malondialdehyde (MDA) assay was found to be reasonably less when treated with AA-Ag-FA hydrogel compared to standard (Mega heal). Cytotoxicity of the samples tested through MTT assay and live-dead cell staining shows its nontoxic biocompatibility nature. In our hydrogel scaffold, the bio-degradable agar-agar provides the moist environment; the Ag NPs inside the gel acts as bactericidal agent and fumaric acid facilities the antioxidant and angiogenesis path implicitly.

Biography:

Somnath Ghosh obtained B.Sc. degree in Chemistry (Honors) from University of Calcutta, M.Sc. (Chemistry) from IIT Delhi and PhD from IISc Bangalore. His current research field is on synthesis of biocompatible nanomaterial for antibacterial and wound healing activity and elucidate the mechanism for such bio-activity. He is working at Indian Institute of Petroleum & Energy, Visakhapatnam, India as Assistant Professor.

Externally Modulated Biomaterial Based Nanomedicine for On-demand Sitespecific Imaging and Chemoradiotherapy

Prateek Bhardwaj[1*]
Jayant Sastri Goda[2]
Venkatesh Pai[2]
Pradip Chaudhari[2]
Bhabani Mohanty[2]
Trupti Pai[2]
Komal Vishwakarma[2]
Rahul Thorat[2]
Tabassum Wadasadawala[2*]
Rinti Banerjee[1*]

[1]Indian Institute of Technology Bombay, India
[2]Tata Memorial Centre, India

Abstract

Limited therapeutic gain with neoadjuvant chemotherapy of locally advanced inoperable cancers can be improved with concomitant use of chemoradiotherapy owing to their spatial cooperation and synergistic cytotoxicity. However, poor circulation half-life, limited passive bioavailability, and dose-limiting systemic toxicities of clinically approved radiosensitizers significantly affects the treatment efficacy and patient's quality of life. Incorporation of clinical radiosensitizers into smart biomaterials based nanomedicines can overcome these limitations, however location of the malignant niche is imperative to their rational designing. To target deep-seated malignancies like triple negative breast cancer (TNBC) or metastatic niches, we designed an ultrasound and tumor microenvironment responsive 'stealth' theranostic nanoconjugate platform for contrast enhanced imaging and on-demand spatiotemporal delivery of combinatorial radiosensitizers post systemic administration. Developed strategy imparted site-specific focussed ultrasound mediated infiltration of nano-conjugates at the orthotopic TNBC xenograft in NODSCID mice followed by low pH and hyperthermia dependent release of drugs at the tumor interstitium to ameliorate clinical chemotherapy as well as radiotherapy. Our findings suggest the clinical potential of such malignant niche-specific externally triggered platforms for the efficient management of radioresponsive tumors as well as metastatic niches.

Biography:

Prateek Bhardwaj is a postdoctoral fellow at the Indian Institute of Technology (IIT) Bombay, Mumbai, India. His research expertise primarily includes the development of theranostic platforms using smart biomaterials for cancer. Pertaining to his masters and doctoral research from IIT Bombay, he has been granted a patent and published several peer-reviewed research and review articles in esteemed international journals like Nanoscale, Journal of Controlled Release, Biomaterials, Acta Biomaterialia, and Biomacromolecules. He has shared his research leads through multiple oral talks including 'keynote' talk at different international conferences. His future research interest lies in nano-immunoengineering for oncology.

Bio-Props for Regeneration

Mamatha M. Pillai[1]
H.N. Tran[2]
Shadi Hoshyar[3]
Rajiv Padhye[3]
Insup Noh[2]
Amitava Bhattacharyya[2]

[1]Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, India

[2]Convergence Institute of Biomedical Engineering and Biomaterials, Seoul National University of Science and Technology, Seoul 01811, Republic of Korea

[3]RMIT Microscopy and Microanalysis Facility, College of Science, Engineering and Health, RMIT University, Melbourne 3001, Australia

Abstract

Recent advancements in tissue engineering have proven its potential in the regeneration of tissue using additive manufacturing techniques. 3D printing is a promising technique for the development of scaffolds with biomimetic properties that provides a proper microenvironment for cell proliferation as well as tissue regeneration. Nanocellulose pellicle is produced as a byproduct during the symbiotic culture of bacteria and yeast in kombucha. However, it has limited application in tissue engineering due to its low processability. In this work, bacterial cellulose-based sustainable kombucha (KBC) sheet has been produced and it was acid-treated to partially hydrolyse. This controlled process improves its extrusion and shape formation ability. The physical, functional and biological properties were studied to assess its potential as a 3D printed scaffold for wound healing. We have also designed a new nanocomposite material composed of dopamine, carbon nanofibers (CNF) and polycaprolactone (PCL) for the fabrication of nerve conduits, which facilitates the growth and migration of neurons toward the targeted end of an injured nerve. The in vitro cell study of human glioma cells showed that the printed lines provided support for neural cell attachment, migration and differentiation toward the targeted end. In contrast, in the absence of printed lines in the scaffold, the cells attach and grow in random directions, forming a flower shape (cell cluster) on the surface of PCL. Thus, the proposed scaffold is a promising candidate for nerve guide application based on its signal transmission and navigating neurons in a correct pathway towards the targeted end.

Biography:

Mamatha M. Pillai is currently a Postdoctoral Fellow in the Cell and Tissue engineering Lab at IIT Bombay. She completed her Ph.D. in Nanobiotechnology from PSG Institute of Advanced Studies, Coimbatore, Tamil Nadu. Her major research interests are biomaterials, tissue engineering and regenerative medicine. She has research experience in biomaterial synthesis, scaffold development using various techniques such as electrospinning, cryogelation and 3D printing. She has 42 publications, several patents, and awards to her credit.

A New Concept on Ceramic Adsorbent Preparation for Defluoridation of Ground Water

Sunipa Bhattacharyya[1*]
Amit Kumar Yadav[1]

[1]Department of Ceramic Engineering, National Institute of Technology Rourkela, Sundargarh, Odisha-India

Abstract

The present research unveils a simple process of preparing bead-shaped porous ceramic adsorbents for mitigating excess fluoride ions from groundwater. The bead-shaped adsorbents were prepared using the acid leachate of a low-cost, readily available ceramic raw material, kaolinite. Here acid leachate act as a starting solution, and the process followed is the oil-drop method. The effect of different parameters on the formation, morphology and stability of the prepared ceramic adsorbents were studied and reported. The porous network is incorporated in the bead-shaped adsorbents by using organic pore former. The formed adsorbents were initially aged, dried and then fired at different temperatures to get the desired ceramic phases. Characterization of the prepared adsorbents was done by powder X-ray diffractometer (XRD), thermogravimetry (TG), differential scanning calorimeter (DSC), Fourier transforms infrared spectrophotometer (FTIR), field emission scanning electron microscope (FESEM), N2 adsorptiondesorption surface area analyzer and a pore size analyzer. The pore size distribution study confirmed the porous nature of the beads as per the Barrett, Joyner, and Halenda (BJH) method and FESEM images. These adsorbents' porous nature and higher surface area predict their suitability for defluoridation of fluoride contaminated groundwater. The bead shape instead of powder ensure their easy separation after use.

Biography:

Sunipa Bhattacharyya works at the Department of Ceramic Engineering faculty, National Institute of Technology, Rourkela. She has more than ten years of experience in teaching and research related to Ceramics in Academics. She got various awards all through her carrier for academic performances and research contributions. Her fields of interest are structural ceramic, porous ceramic adsorbents and waste recycling. Prof. Bhattacharyya has 24 SCI journals publications and 6 conference papers. Presently two students are continuing PhD research under her supervision. She is involved in sponsored research and attached as a reviewer with many journals in Ceramic materials.

Interesting Perspective of the Aurivillius Phase of Ferroelectric Oxides for Memory Device Application

B. Harihara Venkataraman*

Department of Physics, Birla Institute of Technology and Science (BITS) - Pilani, Hyderabad Campus, Jawahar Nagar, Kapra Mandal, Hyderabad - 500078, Telangana State, India.

Abstract

The Aurivillius families of ferroelectric oxidessuch as SrBi2Ta2O9 (SBT), BaBi2Nb2O9 (BBN) and Bi4Ti3O12 (BIT) have been widely used in piezoelectric, pyroelectric and nonvolatile random access memory (NVRAM) devices. These materials have interesting inherent characteristics like fatigue-free behaviour and low coercive field. However, it possesses low remnant polarization, high processing temperature and high dc conductivity which has been considered a hindrance for the better performance of NVRAM devices. On the other hand,

the physical properties of these Aurivillius families of ferroelectric oxides could be tailored by doping the suitable cations in the crystal lattice of $Bi_4Ti_3O_{12}$ and $SrBi_2Nb_2O_9$ ceramics. Interestingly, the lanthanum ion doped bismuth titanate profoundly influenced the physical properties especially dielectric and ferroelectric. Keeping this view in mind, we have substituted Bi^{3+} by Sm^{3+} in the crystal lattice of SBT and BBN layered ferroelectric materials synthesized by low temperature molten salt method using KCl as a flux and studied its influence on the microstructural, dielectric and ferroelectric properties to exploit these materials specifically for NVRAM devices. The presentation shall highlight the important aspects of bismuth oxide - based layered ferroelectric materials and also the investigations on the influence of samarium ion doping on the physical properties of these ceramics will be discussed.

Biography:

B. Harihara Venkataraman is an Associate Professor in the Department of Physics, BITS - PILANI, Hyderabad Campus, Hyderabad, India. He was awarded Ph.D in Materials Science by Indian Institute of Science, Bangalore, India in 2006. He was a post-doctoral researcher at Nagaoka University of Technology, Nagaoka, Japan from June 2006 to September 2008. He was awarded “Centre of Excellence Fellowship” for his post - doctoral programme in Japan. He received “Young Scientist Fast Track Project” from the Department of Science and Technology, India. He has research expertise in glass/polymer nanocomposites, laser writing in glasses and structure - property correlation studies in ferroelectric and multiferroic materials. He has published several research articles in refereed journals with a book chapter on multifarious transparent glass nanocrystal composites and also presented his work in various reputed national and international conferences. He is a member of Institute of Electrical and Electronics Engineers (IEEE), Magnetic Society of India (MSI) and Materials Research Society - Singapore (MRS - S).

Towards Development of Tailored Energetic Materials Utilizing the Chemistry of Coordination Polymers

Saona Seth

Department of Applied Sciences, Tezpur University, India

Abstract

The area of energetic materials is as old as the subject ‘Chemistry’. Energetic materials are compounds or formulations that typically contain intimately mixed oxidizing and fuel components, such that they can undergo self-sustained combustion with release of energy in the form of heat or light when initiated by suitable external stimuli. An ideal energetic material should also display good thermal stability, controllable impact sensitivity, high density, and produce environmentally benign reaction products upon detonation. These requirements point to the potential advantages of CP tunability in producing tailored energetic materials. We adopted several approaches to develop high density, and insensitive energetic materials (secondary explosives) utilizing the chemistry of CPs. One strategy was to employ coordination polymerization of known organic energetics to investigate how metal-coordination can influence its energetic parameters. It was observed that coordination polymerization leads to dense network structures with high crystallographic densities in which, the deprotonated organic energetic compounds are thermally desensitized. Furthermore, it was also demonstrated that coordination polymerization of an organic energetics might

result in improved oxygen balances and tunable sensitivities to external stimuli depending on the constituent metal ions. In another approach, high-energy materials were synthesized by loading oxidizer guests in a porous MOF that serves as a fuel. The resulting energetic composites contain intimately mixed oxidizer-fuel components; such molecular level mixing is crucial for rapid and efficient reaction.

Biography

Saona Seth obtained M.Sc and Ph.D in Chemistry from Indian Institute of Technology Kanpur, India. After pursuing her postdoctoral research with Prof. Adam J. Matzger at the University of Michigan and Prof. M. G. Finn at Georgia Institute of Technology, she joined Tezpur University, India as an Assistant Professor of Chemistry in the Department of Applied Sciences. Her research interest encompasses developing porous organic and metal–organic polymers for different applications. She has received a number of national level recognition in India, viz. National Merit Scholarship, Shyama Prasad Mukherjee Fellowship, etc.

Metallization Degree and Metallic Iron Content of Hematite Ore Using Non-Contact Direct Reduction Method

J.E. Ogbezode[1,2*]
O.O. Ajide[1]
O. Ofi[1]
O.O. Oluwole[1]

[1]Department of Mechanical Engineering, University of Ibadan, Ibadan, Nigeria.

[2]Department of Material Science and Engineering, African University of Science and Technology, Abuja, Nigeria

Abstract:

The problem associated with the scarcity of coking coal in the production of direct reduced iron (DRI) and the effect of carbon deposition in iron production which in-turn affect their manufacturing properties cannot be overemphasized. Thus, this paper attempts to use non-coking coal (charcoal) as an alternative carbon-bearing material for the reduction of goethite-hematite ore acquired from run-off mines, fired at an isothermal temperature of 570-10000C at residence time of 6mins in an activated carbon furnace. The morphological and microstructural phases of the sample were analyzed at the pre-reduction and post-reduction stages using XRD, XRF, and SEM/EDX Micrograph. Results revealed a DRI with a metallization degree of 93% and metallic iron content of 61.7% respectively. The method employed is the novel non-contact direct reduction method which implies that the non-contact reduction method can serve as an alternative DRI production route instead of the conventional direct reduction process of iron ore, with little or no trace of carbon deposition.

Biography:

Engr. OGBEZODE is currently conducting his research on Comparative Analysis of Goethite-Hematite Ore Using Reducer-Smelting Process as alternative route for Iron and steelmaking process in order to minimize furnace energy consumption and carbon deposition. OGBEZODE completed his bachelor's degree in Mechanical Engineering from University of Ibadan and obtained his Master's degree in Mechanical Engineering from the same University. OGBEZODE serves as a Lecturer/Research Associate at Edo State University Uzairue, Edo State, Nigeria, engaging on teaching-learning, conducting research and serving the community. He specializes in Material Development, Applied Mechanical and Extractive Metallurgy. Moreover, he is well published author in reputable journals (both local and international).

Bio-Functional Multi-Layers Deposited on the Surface of Ti-Based Alloys with Chemical Plasma Treatment for Bioengineering

Karol Kyzioł*

AGH University of Science and Technology, Faculty of Materials Science and Ceramics, A. Mickiewicza Av. 30, 30 059, Kraków, Poland

Abstract

The research is focused on the intentional surface modification imparting the particular physicochemical and useful properties to NiTi and Ti6Al7Nb alloys. All surface functionalization approaches involved plasma treatment in the PE RF CVD (Plasma Enhanced Radio Frequency Chemical Vapour Deposition) system and subsequent deposition of biopolymers-based coatings. Two different types of multi-layers: 1) nanocomposite layers of chitosan enriched with Ag and/or Au nanoparticles and 2) chitosan layers with caffeic acid covalently inserted onto polymer backbone or physically embedded into polymer matrix were proposed. The resulting functionalized substrates were precisely characterized by techniques adequate for materials engineering such as SEM-EDS analysis, AFM, optics profilometry, IR and Raman spectroscopy, wettability, ICP-MS and nanoindentation method, corrosion test. Noteworthy, the influence of all surface modifications on the different surface parameters such as roughness, hydrophilicity, surface energy, delamination, and as well on the biocompatibility and bacteriostatic/bactericidal activity were examined in detail. Moreover, a comparative study of the biological response of the surface modified alloys towards both prokaryotic and eukaryotic cells in vitro was evaluated.

In general, bio-functional multi-layers deposition on the surface of Ti-based alloys involving plasmochemical approach and biopolymers layer-by-layer (LbL) self-assembly resulted in the construction of bioactive coatings enriched with metal nanoparticles (Ag, Au nanoparticles) or bioactive small molecules (caffeic acid) for bioengineering. Versatility of this approach ensures functionalities with improved physicochemical properties tailored by controlling the molecular arrangement having nanoscale precision.

Acknowledgements: This work was supported from the subsidy of the Ministry of Education and Science for the AGH University of Science and Technology in Kraków (Project No 16.16.160.557).

Biography:

Karol Kyzioł is Professor at AGH in the field of Materials Engineering, Head of the Department of Physical Chemistry and Modelling and Head of Laboratory of Vapour Deposited Materials.

His academic achievements consist of 120 published scientific publications, including 35 papers (Journal Citation Reports) with the total IF ca. 95. Prof. Kyzioł is also the co-author of two book chapters (Published by Wiley-Scrivener and Elsevier) and co-author of two patents.

3D Scaffolds as Artificial Lymph Nodes for Cancer Immunotherapy

Judith Guasch[1,2,3*]
Eduardo Pérez del Río[1,2]
Fabião Santos[1,2]
Miquel Castellote-Borrell[1,2]
Imma Ratera[1,2]
Jaume Veciana[1,2]

[1]Institute of Materials Science of Barcelona (ICMAB-CSIC), Spain

[2]Networking Research Center on Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), Spain

[3]Dynamic Biomaterials for Cancer Immunotherapy, Max Planck Partner Group, ICMAB-CSIC, Spain.

Abstract

Adoptive cell therapy is an emerging alternative to regular procedures in cancer treatment that consists of using immune cells as drugs, conferring to patients potential long-term protection. Usually, the therapy consists of extracting autologous T cells from patients, followed by a specific selection or genetic modification of these cells to increase their effectivity against cancer, such as the introduction of chimeric antigen receptors (CARs). Then, these specific T cells are largely expanded and finally reinfused to the patients to act as living drugs. These personalized treatments therefore require laborious and expensive laboratory procedures that should be alleviated to enable their broad use in the clinics. With the objective to improve the ex vivo expansion of therapeutic phenotypes of human (CAR) T cells, we used different 3D biomaterials to mimic the extracellular matrix (ECM) of the lymph nodes, consisting of polystyrene scaffolds and hydrogels. Different improvements in T cell proliferation, differentiation, and function have been observed depending on the used matrix.

Biography:

Guasch is a tenure-track "Ramón y Cajal" researcher at the Institute of Materials Science of Barcelona (ICMAB-CSIC; Barcelona, Spain) and the head of a Max Planck Partner Group (Dynamic Biomimetics for Cancer Immunotherapy, https://dynamic-biomimetics.icmab.es/) in collaboration with the Max Planck Institute for Medical Research (Heidelberg, Germany). She is focused on the design, synthesis and fabrication of novel bionanomaterials for biomedical applications, especially those related to cancer research.

Precise Quantification of Calcium and Phosphorous Ratio in Apatite's for Routine Analysis

Arturs Viksna[1*]
Karlis A. Gross[2]
Vladlens Grebnevs[1]

[1]University of Latvia, Riga, Latvia

[2]Riga technical university, Riga, Latvia

Abstract

Calcium phosphates as essential materials in different fields, and in implants offer unique properties and thus need accurate control of the composition. Hydroxyapatite, is the most commonly used member of the calcium phosphates; the ability to accommodate defects and substitutional elements accentuates the importance for a precise quantification of the

calcium and phosphorous content. Several methods are available for assessing the chemical composition, but these have not been compared for the routine quantification of apatites. The first assessment of purity is usually expressed as a Ca/P molar ratio. This single quantitative measure of both the calcium and phosphorous content has been adopted as a standard reporting unit.

Nowadays, ICP-OES and photometry are used more commonly; gravimetry. titrimetry, XRD and FAAS are used less. These methods are well-established and easily accessible, but there are some limitations and difficulties (high analysis cost or time consuming or luck of reference materials or single element method) for an effective introduction into a routine analysis practice of calcium phosphates. TXRF offers simple sample preparation, has a relatively short analysis time, allows multi-element determination to a relatively high degree of accuracy, offers semi-quantitative determination of inorganic impurities, has low hardware maintenance costs, requires a small sample size, and does not require expensive reagents. A portable benchtop TXRF available in the instrumentation market which is attractive for calcium and phosphorus routine analysis in the quality control labs. It can be concluded that quantification results of TXRF analysis were in a good agreement and somewhat superior to other modern and classical methods.

Biography:

V. Grebnevs, L. Busa, L. Pluduma, A. Viksna, K.A. Gross. Comparison of different classical and instrumental analysis methods for precise quantification of calcium and phosphorous ratio in hydroxyapatite, Key Engin. Mater. 800 (2019) 47-51. https://doi.org/10.4028/www.scientific.net/KEM.800.47

Building Competitive Bone Biomaterials by Self-Assembly of Collagen/Apatite

Nadine Nassif*

*Sorbonne Université, CNRS, Collège de France, Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP), 4 place Jussieu, F-75005, Paris, France.

Abstract

In biological tissues, a common feature is the presence of dense arrays of biopolymers with ordered geometries at the ultrastructural level. A relationship was established between such 3D arrangements formed by the biological polymers and molecules in liquid crystals (see publications of Y. Bouligand). This structural analogy between living tissues and liquid crystals suggests similar self-assembly mechanisms in both systems. For Type I collagen (the major structural protein of connective tissue), liquid-crystal self-assembly was shown through the observation of a cholesteric phase in a highly concentrated state in vitro. After a sol/gel transition, collagen fibrils were formed while preserving the cholesteric geometry (see publications of M.M. Giraud-Guille).

Recently, the samples were scaled up (from drop to bulk material) using a process based on a continuous injection of collagen to increase the protein concentration. Coupling the liquid-crystalline properties of collagen to a bioinspired hydroxyapatite mineralization process leads to the synthesis of a collagen/apatite composite with high similarities with the bone tissue in terms of composition and structure. We will show that the resulting materials provide original models to study fundamental questions on tissue morphogenesis and, more particularly, bone

biomineralization and the role of collagen liquid-crystal domain during bone tissue formation. In vitro and in vivo investigations were performed to control their cyto- and biocompatibility and to evaluate their potential for bone repair. They are found to be a good starting point for applications in bone tissue engineering through the design of new implantable materials since autologous bone is still considered as the gold standard.

Biography:

Nadine Nassif is a CNRS researcher at the Laboratory "Chimie de la Matière Condensée de Paris" (UMR 7574). Her research focuses on collagen self-assembly to biomimetics materials for tissue engineering and biomineralization studies. She completed her professional qualification (Habilitation) in 2016 on "physico-chemical approaches of bone biomineralization". Her main present interest is building a tissue library based on Type I collagen self-assembly by controlling the three-dimensional shaping of the resulting materials and determines the "structural-function" properties to build competitive biomimetic (bio)materials.

Generation of Ovarian Tumor Spheroids and Invasion on-a-Chip

Changchong Chen[1]
Ambroise Lambert[2]
Yong Chen[1]
Carole Aimé[1*]

[1]PASTEUR, Département de chimie, École Normale Supérieure, PSL University, Sorbonne Université, CNRS, 75005 Paris, France

[2]ERRMECe, Equipe de Recherche sur les Relations Matrice Extracellulaire-Cellules (EA1391), Université de Cergy-Pontoise, 95001 Neuville sur Oise Cedex, France.

Abstract

Progress in cancer research relies partially on our ability to provide relevant in vitro models, which recapitulate important features of tumor growth and metastasis. We developed an invasion assay by using microfabricated culture devices. First, ovarian tumor spheroids were generated with a culture device consisting of an agarose membrane on a gelatin nanofiber backbone. We show how to tune the number of cells in, and the size of the spheroids so as to reproduce metastasis evolution during different stages of ovarian cancer. Second, another microfabricated culture device was coated with extracellular matrix proteins to tune the topology, the stiffness and the adhesion properties of the substrate. We use a combination of type I and type IV collagen and laminin to recapitulate both connective tissues and basal membrane. This device effectively allows to monitor the invasive behavior of SKOV-3 human ovarian cancer cells in the chip providing a unique insight into cells transitioning within the epithelial to mesenchymal transition spectrum. Finally, by the integration of the two culture devices into microfluidic chips, we can form a close loop to simulate the tumor microenvironment and apply different stimuli such as shear stress, growth factors, and drugs. This on-chip process is straightforward and spheroid type independent and should be applicable to other cancer types, as well as assays under microfluidic conditions, thereby holding the potential for use in tumor modeling and anti-cancer drug development.

Biography:

Carole Aimé is a CNRS researcher working at the Chemistry Department of the Ecole Normale Supérieure in Paris-France. After a PhD in Bordeaux University-France, on self-assembling amphiphilic systems, she joined Kyushu University-Japan, where she designed functional coordination nanoparticles from nucleotides and lanthanide ions. She got a CNRS position working on the engineering of biomaterials and bionanocomposites combining inorganic nanoparticles with collagen at the Laboratoire de Chimie de la Matière Condensée de Paris-Sorbonne University-France. She moved to ENS in 2018 to develop integrative in vitro models for biological and biomedical research.

Biomimetic Approach to Investigate the Effect of Heparan Sulfate on BMP2-Mediated Osteogenic Differentiation

Julius Sefkow-Werner[1,2]
Jean Le Pennec[2]
Paul Machillot[2]
Catherine Picart[1,2,3]
Elisa Migliorini[2*]

[1]Univ. Grenoble Alpes, CNRS, Grenoble INP**, LMGP, 38000 Grenoble, France [3] CEA, direction of fundamental research, interdisciplinary research institute of Grenoble (IRIG), FRE CNRS, Grenoble, France

Abstract

Over the last decade there has been a growing interest in the development of new materials to improve bone morphogenetic proteins (BMPs) delivery for tissue regeneration. In vivo, BMP2, 4, 6 and 7 are bound to extracellular matrix (ECM) components, mostly to fibronectin and heparan sulfate (HS) and with less extent to chondroitin sulfate (CS). The development of materials which are able to control BMPs molecular presentation by mimic its in vivo presentation is an essential approach for a deeper understanding of BMPs functions and the modulation of its biological activity.

We develop and apply model surfaces that co-present grafted adhesion peptides (cRGD) with immobilized BMP2 alone or adsorbed to HS. The binding of each component on these biomimetic surfaces is highly controlled, in terms of stoichiometry of molecules and BMP2/grafted-HS affinity, as determined by surface sensitive techniques1. The amount of cRGD peptides can be tuned to affect cellular adhesion. The functionalization of these platforms have also been automated to decorate an entire 96 wellplate with different conditions. Functional validations of the surfaces are performed using a murine myoblast cell line (C2C12) and human periosteum derived stem cells (hPDSCs).

Grafted HS permit BMP-SMAD signaling in a dose-response manner 2. In particular, HS positively affects BMP2-mediated osteogenic differentiation3, suggesting a potential importance of ECM-HSPGs as regulators of BMP2 activity. These highly versatile platforms could be applied to many other HS-binding proteins to study their role on cell signaling.

Biography:

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How Does the Addition of Birch Tar to PLA and PCL Biodegradable Polymer Materials Change their Properties? - Characteristics of New Eco-Materials.

Agnieszka Richert[1*]
Ewa Olewnik-Kruszkowska[2]
Grażyna B. Dąbrowska[1]

[1]Nicolaus Copernicus University in Toruń, Department of Genetics, Faculty of Biology and Veterinary Science, Lwowska 1, 87-100 Toruń, Poland.
[2]Nicolaus Copernicus University in Toruń, Chair of Physical Chemistry and Physicochemistry of Polymers, Faculty of Chemistry, 7 Gagarina Street, 87-100 Toruń, Poland.

Abstract

The main objective of this study was to use the oldest substance used by man over the centuries to produce eco-materials based on PLA and PCL biodegradable polymers. A bactericidal film was produced, which was done for the first time according to the literature analysis. The obtained polymer films consisted of PLA, PCL, birch tar (1-10%) and the addition of a plasticizer in the amount of 5% by weight. % PEG. Materials based on PLA and PCL were tested in terms of morphology (SEM, AFM), spectrophotometry (FTIR), water vapor permeability (Pv), strength properties, and antibacterial properties. It was found that the introduction of tar to PLA and PCL leads to materials with satisfactory biological and functional properties, as well as physicochemical and structural properties, which classifies this material into a wide range of application possibilities.

The project “Innovation Incubator UMK_4.0 under the program of the Ministry of Education and Science entitled “Incubator of Innovation 4.0” (no. MNISW/2020/331/DIR) as part of a non-competitive project entitled “Support for the management of scientific research and commercialization of R&D results in research units and enterprises”, implemented under the Intelligent Development Operational Program 2014-2020 (Measure 4.4), co-financed by the European Regional Development Fund.

Biography:

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2. Richert, A., Dąbrowska, G.B., Dąbrowski, H.P., 2020. Bactericidal polylactide film and the method of its preparation. Patent Application P.433979 (in Polish)

Fracture in SiO2-B2O3-Na2O Glasses

Cindy L. Rountree[1*]
Weiying Feng[1]
Daniel Bonamy[1]
Fabrice Célarié[2]
Paul C. M. Fossati[3]
Stéphane Gossé[3]
Patrick Houizot[2]
Michel Mama Toulou[1,3]

[1]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

[2]Université Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France

[3]Université Paris-Saclay, CEA, Service de la Corrosion et du Comportement des Matériaux dans leur Environ-nement, 91191, Gif-sur-Yvette, France

Abstract

During 2022, the global market for flat glass is estimated to exceed 100 billion metric tons. Moreover, the glass industry concerns many sectors of our daily lives (buildings, cars, dishes…) along with being integral parts of heat resistant technologies, protection panels (smart phones, plasma screens…), low-carbon energies (protection for solar panels) and satellites in outer space to name a few. Making them less reactive to Stress Corrosion Cracking (SCC), tougher (increasing their fracture toughness, Kc) and lighter, while maintaining other properties, is a fundamental issue plaguing glass scientists and researchers.

This presentation will take a closer look on how the chemical composition of SiO2-B2O3-Na2O ternary glass systems alters the physical, mechanical and fracture properties of these systems. These changes lead to mesoscale changes as revealed by a novel parameter coined the depolymerization index. This parameter reveals surprising trends with the stress corrosion cracking behavior in Region I. The presentation will focus on stress corrosion cracking and how it varies with chemical composition and the depolymerization index.

Biography:

Cindy L. Rountree is a senior research scientist in SPEC at the Université Paris-Saclay, CEA, CNRS where she has worked since 2006. She has distinguished herself as a specialist of the nanoscale mechanisms associated with static and dynamic fracture propagation in brittle materials. She is currently studying stress corrosion cracking in SiO2-B2O3-Na2O ternary glass systems.

Novel Biodegradable FeMn-Based Alloy for Additively Manufactured Implants

Julia K. Hufenbach[1,2*]
Martin Otto[1]
Birgit Paul[1]

[1]Leibniz Institute for Solid State and Materials Research Dresden, Institute for Complex Materials
[2]Technische Universität Bergakademie Freiberg, Institute of Materials Science

Abstract

Additive manufacturing of biodegradable alloys for patient-specific implant applications is currently drawing increasing attention. Laser powder bed fusion (LPBF) presents an excellent

technology to fabricate near-net-shape structures out of biodegradable metals. Thereby, Fe-Mn-C-based alloys are considered as interesting candidates for biodegradable stents due to their high strength, ductility, and mechanical integrity during degradation. This work presents the successful processing of a novel Fe-30Mn1C-0.02S (FeMnCS) twinning induced plasticity alloy by LPBF. The high solidification rate during this process causes a fine austenitic microstructure with homogeneous element distribution, which results in largely uniform corrosion and in attractive mechanical properties in comparison to a conventional corrosion resistant AISI 316L steel. Thereby, an effect of the build orientation on microstructure and mechanical properties of compact samples could be detected. In addition, filigree degradable FeMnCS stent structures were built by LPBF and mechanically evaluated. Furthermore, the initial cell-material interactions were examined (in comparison to LPBF-processed 316L). Different corrosion stages of the stent surfaces were simulated by pre-conditioning in DMEM under cell culture conditions for 2 hours, 7 days, and 28 days. Subsequently, human umbilical vein endothelial cells were directly seeded onto the pre-conditioned samples and the cell viability, adherence and morphology were analyzed. In contrast to the short pre-conditioning, the cells seemed to proliferate after 7 and 28 days of pre-conditioning for up to 14 days. This can be traced back to the formed degradation layer inhibiting ion release. Concluding, the novel alloy shows a high potential for future application as biodegradable implant material.

Biography:

Julia Hufenbach received her diploma in "Materials Science and Technology" from the TU Bergakademie Freiberg (Germany) in 2010 with distinction. Afterwards, she started her doctoral studies on tool steel development at Leibniz Institute for Solid State and Materials Research (IFW) Dresden in tandem with TU Dresden and obtained her doctoral degree (with distinction) in 2014. After a Postdoc position at KITECH, Korea, she became group leader at IFW Dresden and intensified her research activities on biodegradable alloys. In 2019, Julia Hufenbach was appointed as Professor for Materials Functionalization at TU Bergakademie Freiberg and division leader at IFW Dresden.

Evaluation of Essential Oil Loaded Fibrous Mats Against the Escherichia Virus MS2, a Mimic of SARS-CoV-2, for Protective Face Mask Uses.

Helena P. Felgueiras

Centre for Textile Science and Technology, University of Minho, Campus de Azurém 4800-058 Guimarães, Portugal

Abstract

Face mask usage is one of the most important measures to reduce SARS-CoV-2 transmission. Yet, most masks display a passive-like action. Here, we propose to overcome this limitation by incorporating antiviral essential oils (EOs) within polycaprolactone (PCL) electrospun fibrous mats. Twenty EOs were examined for the first time against the Escherichia coli MS2 virus (potential surrogate of SARS-CoV-2). The most effective were the lemongrass (LGO), Niaouli (NO) and eucalyptus (ELO) with a virucidal concentration (VC) of 356.0, 365.2 and 586.0 mg/mL, respectively. PCL was processed via electrospinning and EOs were loaded via: (1) physisorption on pre-existing mats (PCLaEOs), and (2) EOs blending with the polymer prior to fiber extrusion (PCLbEOs). In both cases, 10% VC was used as loading concentration. EOs presence and release from mats was confirmed by UV-visible spectroscopy (≈5257-631 μg) and gas chromatographymass spectrometry (≈14.3% EOs release over 4 h), respectively. PCLbEOs

mats were considered the more mechanically and thermal resilient, with LGO promoting the strongest bonds with PCL. Mats modified with the EOs were all identified as superhydrophobic. Air and water-vapor permeabilities were affected by the mats' porosity (PCL<PCLaEOs1). The most effective combination against the MS2 viral particles was the PCLbLGO. These mats were also deemed the most pleasant during sensory evaluation. Overall, data demonstrated the potential of these EOs-loaded PCL fibrous mats to work as COVID-19 active barriers for individual protection masks.

Biography:

Helena Felgueiras is a Biomedical Engineering from University of Minho (Portugal) with a PhD in the same field (specialization in biomaterials) from Université Paris 13 (France). Presently, she works has a Junior Researcher at the Centre for Textile Science and Technology (2C2T, Portugal), developing antimicrobial surfaces resorting to biological cues, and heading the line of research in medical textiles. She is the author of 55 publications, with a h-factor of 16 (Scopus). HF has international collaborations with 10 countries, reflected in published work (85 co-authors). She has given 108 national/international communications and has received 9 awards and 24 distinctions.

Study of Ecological Materials and Additive Manufactured Structures as a Substitute of Expanded Polystyrene Foams

Ramon Miralbes[1*]
Laura Diago[1]
David Ranz[1]

[1]Department of Design and Manufacturing / University of Zaragoza, Spain

Abstract

Expanded polystyrene foam (EPS) is extensively used in energy absorption applications such as packings of goods and helmets due to its low density and high capability to absorb energy. Additionally, this material can by tailed controlling the expansion process in the manufacturing process that controls the final density of the foam. It is well-known that the mechanical properties of EPS (stress levels, strain, energy abortion, etc.) depends on the density. However, EPS manufacturing process only allows to generate foams with only one density.

Recent studies have demonstrated that, to improve the mentioned energy absorption applications, it is necessary to implement materials with different densities depending on the zone that should be protected (i.e. in helmets, different strength of the different zones of the skull and the different tolerance to damage of the different parts of the brain imply the necessity of materials with different mechanical properties). Additionally, EPS is a petroleum based materials with a high carbon footprint.

On the one hand, this article studies the application of ecological materials such as cork, cork agglomerates, luffa and micellar materials in this application to reduce carbon footprint. On the other hand, this article explores the use of additive manufacturing process (AM) to create materials with different densities and different mechanical properties that would be use to optimize energy abortion in the mentioned applications. Hence, it has been compared the main mechanical properties of different densities EPS, different natural materials and lattice AM structures.

Biography:

Ramon Miralbes Buil is professor at the University of Zaragoza since 2008. He obtained his Bachelor degree in 2005 in Industrial Engineering and his PhD in 2008. He is author of more than 30 JCR articles and 50 articles in congress. He has worked in two CE projects, in 5 Spanish projects and more than 20 projects with different companies. He is also reviewer of projects for the CE government. His research area is centered in the mechanical characterization of ecologic materials such as cork, luffa and micellar materials and in the characterization of lattice structures generated by additive manufacturing.

Glass Foams from Waste Materials

Andrea Simon[1*]
Isaac Tsiwah[2]
Chaima Sayari[3]
Masoud Osfori[4]
Tarik Zirari[5]
Meriem Sassi[6]

University of Miskolc, Faculty of Materials Science and Engineering, Institute of Ceramics and Polymer Engineering

Abstract

Glass foams are one of the most promising candidates in the recycling opportunities of several waste materials. Their preparation method is considerably easy via the pressing-sintering route. Besides converting waste materials into a secondary raw material, they have several advantageous properties as good insulation (low thermal conductivity), low density, and good specific strength. In this research work, glass foams were prepared completely from waste materials. The foaming behavior of the mixtures was characterized by heating microscopy to find the optimal sintering temperature. The density, thermal conductivity, and compressive strength of the foams were tested to reveal the effect of waste materials on the properties of the foamed products.

Biography:

Andrea Simon works as an associate professor at the University of Miskolc. With her MSc and Ph.D. students, she researches the recycling methods of waste materials, with a special focus on converting these materials into secondary raw materials for the products of ceramic and silicate industries.

Growth of Intermetallic Layer in Twin-roll Cast Clad Aluminium-Steel Sheet

Michaela Šlapáková[1*]
Barbora Křivská[1]
Klaudia Fekete[1]
Rosslav Králík[1]
Peter Minárik[1]
Olexandr Grydin[2]
Mykhailo Stolbchenko[2]
Mirko Schaper[2]

[1]Charles University, Faculty of Mathemacs and Physics, Czech Republic

[2]University Paderborn, Faculty of Mechanical Engineering, Germany

Abstract

Aluminium-steel clad material fabricated by twin-roll casng [1] is a promising material combining advantageous properes of both co-materials – good corrosion resistance and light weight of aluminium and strength of steel [2]. Properes of the final product are governed by the intermetallic layer of Al5Fe2 phase, which forms at the interface during heat treatment [3]. Observaons in scanning electron microscopy revealed that the intermetallic layer between aluminium and steel emerges a?er annealing around 500 °C and grows preferenally towards aluminium. This is in accordance with findings of other researchers (e.g. [4]) and corresponds to the fact the diffusion coefficient of Fe in Al is considerably higher compared to diffusion coefficient of Al in Fe. However, during in-situ heang in transmission electron microscope an intermetallic phase pervades towards steel due to surface effects, making the in-situ TEM observaons non-informave in this case. Observaons of un-polished annealed sample in SEM confirmed the surface-growth of the layer towards steel. The kinecs of the intermetallic phase growth follows the parabolic law.

Biography:

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Optimization of the Heat Treatment of a Turbine Disc Nickel Superalloy

Magnus Anderson[1*]
Lucia Scotti[1]
Sergiu Pantis[1]
Andrew Rowe[2]
Jonathan Wells[3]
Hector Basoalto[1]

[1]The University of Sheffield, United Kingdom

[2]RWE, United Kingdom

[3]Risktec Solutions, United Kingdom

Abstract

Mean-field precipitation models have reached a maturity where they are able to successfully guide the design of heat treatments of new nickel superalloys, reducing the amount of experimentation and time-consuming characterisation, and accelerate the alloy design process. It is possible to tailor the precipitate dispersion for specific properties considering yield strength, fatigue life, or creep resistance. To predict this behaviour requires the direct linkage between the precipitate dispersion and plastic response.

This work presents recent advances in calculating precipitate strengthening accounting for a multi-modal dispersion. This is combined with a mean-field model predicts the kinetics of the tertiary precipitate dispersion, enabling the identification of potential heat treatments that can optimise specific mechanical properties.

Biography:

Magnus Anderson is a lecturer in Metallurgy at the University of Sheffield, working within the multi-scale materials modelling team. He specializes in statistical modelling of solid-state precipitation utilising chemical thermodynamics. The models developed have passed key technology readiness levels within their industrial partner and have won an international award for predictive capability in the 2018 AM Benchmark challenge organized by NIST and TMS.

Development of Graphene Oxide/Epoxy Composites by Means of Epoxy/Thiolene Photopolymerization

Ricardo Acosta Ortiz*
José de Jesús Ku Herrera
Aida Esmeralda Garcia

Valdez Centro de Investigación en Química Aplicada, Saltillo, Mexico

Abstract

This talk deals with the development of graphene oxide (GO)/epoxy composites by means of the epoxy/thiol-ene photopolymerization technique. This method presents advantages such as high reactivity, obtaining the composites in minutes, in comparison with hours that require the conventional thermal curing of epoxy/graphene composites; in-situ reduction of GO to obtain rGO/epoxy composites; and improved toughness of the obtained materials due to presence of the flexible species such as the polythioethers in the polyether-polythioether

crosslinked co-network derived from the epoxy/thiol-ene photopolymerization method. In this technique an epoxy resin is cured by the action of a thiol-ene system that comprises a tetraallyl functionalized diamine as curing agent, a multifunctional thiol as crosslinker and a radical photoinitiator. Model studies with monofunctional compounds were carried out with the aim to demonstrate the functionalization and reduction of GO during the photopolymerization of the formulation. The epoxy compound 1,2-Epoxy 3-phenoxipropane, the monofunctional thiol 3-methyl mercaptopropionate and the curing agent N, N-diallylhexan-1-amine, were irradiated with UV light confirming that GO was reduced during the irradiation of the photocurable formulations and at the same time functionalized with thiol groups. The formation of covalent bonds between the rGO and the crosslinked polyether-polythioether co-network resulted in an improvement of the mechanical properties of the rGO/composites obtained when multifunctional monomers were employed in the photopolymerization.

Biography:

Ricardo Acosta Ortiz studied Chemistry at the State University of Coahuila in Mexico and graduated as BSc in 1985. He then joined the chemistry research group at the Applied Chemistry Research Center (CIQA). He received a PhD degree at the Manchester Metropolitan University, UK in 1995. After one year postdoctoral fellowship supervised by Prof James Crivello in The Rensselaer Polytechnic Instiutte in Troy, NY in 2000 he obtained the position of senior researcher at CIQA. He has published more than 60 research articles in SCI(E) journals.

Shear Assisted Processing and Extrusion (ShAPE) of Aluminum Alloys 2024 and 7075 Tubing with Reduced Process Energy

Scott Whalen*
Mathew Olszta
Md. Reza-E-Rabby
Timothy Roosendaal
Tianhao Wang
Darrell Herling
Scott Taysom
Julian Atehortua
Miao Song
Joshua Silverstein
Nathan Canfield
Daniel Graff
Mageshwari Komarasamy
Brian Milligan
Tamas Varga
Anil Battu
Anthony Guzman
Nicole Overman

Pacific Northwest National Laboratory, Richland WA, United States of America

Abstract

Shear Assisted Processing and Extrusion (ShAPE) was used to fabricate aluminum alloy 7075 and 2024 tubing with 12 mm outer diameter and 1 mm wall thickness having superior mechanical properties and reduced process energy compared to conventional extrusion. Unlike conventional extrusion where the billet is rammed against a stationary die using a

strictly linear motion, the ShAPE process superimposes a rotational shear force by spinning the die while plunging the billet. Compared to conventional linear extrusion, the ShAPE process imparts significantly more strain into the feedstock material which enables an array of property and process improvements for aluminum alloys. For example, ShAPE extruded 7075-T6 achieved tensile properties which exceed the ASTM standard and ASM typical values, while simultaneously eliminating the need to homogenize billets (430 °C for 24 hours) and pre-heat billets (400 °C) in a separate furnace prior to extrusion. Solution heat treating after extrusion (465 °C for 1 hour) was also eliminated when extruding from homogenized billets yielding a T5 temper with mechanical properties nearly identical to T6. ShAPE extruded 2024-T8510 achieved tensile properties which also exceeds the ASTM standard and ASM typical values. For 7075 and 2024, these property improvements were achieved at extrusion speeds above 7 meters/min compared to the 1-2 meters/min ceiling that is typical of conventional extrusion for these alloys. Microstructure results will be discussed to provide a fundamental explanation for the observed property improvements.

Biography:

Scott Whalen is a Senior Research Scientist in the Applied Materials and Manufacturing Group at the Pacific Northwest National Laboratory. His research interests focus on developing high-shear metals manufacturing processes that reduce energy usage and carbon emissions while providing improved material properties. Alloys of aluminum, magnesium, copper, and bismuth-telluride are currently under investigation by his research teams. He is the recipient of two R&D 100 awards and is a co-inventor on 11 granted and pending patents for Shear Assisted Processing and Extrusion (ShAPE) and is the author or co-author on 29 peer reviewed publications.

Cementitious Composites using Oriented Fibers: Experiences of São Judas Tadeu University

Dimas Alan Strauss Rambo[1*]
Sandro Martini[2]
Marcos Fabrizio Menezes de Freitas[3]
Igor da Silva Brito[4]
Renan Picolo Salvador[5]

[1235]São Judas Tadeu University, Brazil

[4]Mackenzie Presbiterian University, Brazil

Abstract

This work presents results of experimental investigations focused on the magnetic orientation of steel and sisal fibers embedded in cementitious matrices. The work addresses the development of magnetic alignment methodologies and their influence on the mechanical and electrical properties of the resulting cementitious composites. In the first phase, the materials used in the research are presented, as well as two methods for magnetic alignment of fibers: neodymium magnets coupled to a computer-controlled industrial robot and a simplified magnetic circuit using a pair of coils wrapped in a ferromagnetic core. The second phase focuses on the analysis of the electrical and mechanical properties of the composites and assessment of the fiber orientation and positioning. X-ray computed tomography, electrical resistivity and bending tests were used in this phase. The results showed that the projected magnetic systems were able to generate a preferential orientation of the fibers, increasing

the overall mechanical performance of the composites and generating anisotropy on their electrical properties

Biography:

Dimas Rambo has been a professor at the São Judas Tadeu University for the past 5 years and is also the deputy editor of the "Journal of Urban Technology and Sustainability" (e-ISSN: 2675-780X) created at the same institution. It has experience in Civil Engineering with emphasis on cementitious composites, textile and fibrous reinforcement and concretes exposed to high temperatures. Dr. Dimas Rambo received the Award "AEERJ - Dirceu de Alencar Velloso of best doctoral thesis" in civil engineering in Rio de Janeiro (triennium 2014-2017).

Approaches for In-Situ and Operando Characterization of Energy Storage Materials and Systems

Amy C. Marschilok[1,2*]

[1]Stony Brook University, Stony Brook, New York, USA

[2]Brookhaven National Laboratory, Upton, New York, USA

Abstract

Batteries are ubiquitous in our everyday lives and often appear as black boxes. However, the chemistry inherent to their function is diverse and complicated. Some batteries function through insertion processes where the host structure is maintained, where others are based on conversion chemistry where new phases evolve during the electrochemical oxidation-reduction process. Examples of mechanistic insight gained from in situ and operando characterization of electrochemical energy storage materials and systems will be highlighted in this presentation. This will include approaches to spatially locate and resolve insertion and conversion processes, and distinguish productive and parasitic processes in functional energy storage materials and systems.

Biography:

Amy Marschilok is a Associate Professor at Stony Brook University, with a joint appointment as Energy Storage Division Manager at Brookhaven National Laboratory. She serves as Deputy Director for the Center for Mesoscale Transport Properties, an Energy Frontier Research Center funded by the U.S. Department of Energy. Dr. Marschilok was previously employed as a Senior Scientist at Greatbatch Inc., where she was recognized as a Visionary of the Year. Her current research centers on materials and electrode concepts for high power, high energy density, extended life batteries. She has mentored over 50 student researchers and co-authored over 200 publications.

Characterization of 3D Printed Cementitious Auxetic Composites under Flexural Loadings

Tatheer Zahra[1*]
Mohammad Asad[1]
Julian Thamboo[2]

[1]Queensland University of Technology (QUT), Australia
[2]South Eastern University of Sri Lanka, Sri Lanka

Abstract

Auxetic materials inherently have high energy absorption properties due to Negative Poisson's Ratio (NPR) characteristics, which enables them to contract (or expand) in all direction when compressed (or tensioned) along their longitudinal axis. Recent, advances in 3D printing allows rational designing and development of these materials for desired properties. In this research, 3D printed re-entrant chiral auxetic (RCA) geometries by combining the conventional re-entrant auxetic shape and chirality for high NPR and energy absorbing characteristics were developed. Polylactic Acid (PLA) filament which is a sustainable printing filament was used for 3D printing of these geometries. These geometries were then embedded in cementitious matrix as reinforcement to exploit their NPR characteristics to enhance their energy absorption capabilities of cementitious composites. Consequently, three different cell-sizes of RCA geometries were designed to investigate their influence on the overall behaviour of cementitious composites. In total, 36 prismatic composite samples with embedded 3D printed auxetic reinforcement were developed of 20 mm thickness and various widths and lengths. The samples were tested under subjected to bending through three-point loading. The loading rate was also varied from 1 mm/min, 75 mm/min, 150 m/min to 300 mm/min to study behaviour of composites for their application in building protection from high-speed impact loads. The results were analyzed in terms of failure modes, load-displacement curves and energy absorption levels. All RCA geometries exhibited equally to increase the flexural resistance, energy absorption and ductility of cementitious matrix, however, the RCA geometries with larger cell sizes provided enhanced benefit under relatively high-speed loading of 300mm/min.

Biography:

Tatheer Zahra is a Senior Lecturer in Civil Engineering at Queensland University of Technology with a vision to promote innovative engineering materials in construction. Masonry, concrete and auxetic materials are her main research interest areas. Dr Zahra has 7 years of research experience in the field of high energy absorbing auxetic materials and walling structures. She created auxetic materials of high qualities for structural protection against extreme loads such as impact and blast. She is working on improving the ways of producing auxetic composites using 3D printing techniques for convenient manufacturing and application for the safety of structures.

Calibrating the Impressed Anodic Current Density for Accelerated Galvanostatic Testing to Simulate the Long-Term Corrosion Behavior of Buried Pipeline

Yoon-Sik So[1*]
Min-Sung Hong[1]
Jeong-Min Lim[1]
Woo-Cheol Kim[2]
Jung-Gu Kim[1]

[1]School of Advanced Materials Science and Engineering, Sungkyunkwan University, Suwon 16419, Korea
[2]Technical Efficiency Research Team, Korea District Heating Corporation, 92 Gigok-ro, Yongin

Abstract

Various studies have been conducted to better understand the long-term corrosion mechanism for steels in a soil environment. Here, electrochemical acceleration methods present the most efficient way to simulate long-term corrosion. Among the various methods, galvanostatic testing allows for accelerating the surface corrosion reactions through controlling the impressed anodic current density. However, a large deviation from the equilibrium state can induce different corrosion mechanisms to those in actual service. Therefore, applying a suitable anodic current density is important for shortening the test times and maintaining the stable dissolution of steel. In this paper, to calibrate the anodic current density, galvanostatic tests were performed at four different levels of anodic current density and time to accelerate a one-year corrosion reaction of pipeline steel. To validate the appropriate anodic current density, analysis of the potential vs. time curves, thermodynamic analysis, and analysis of the specimen's cross-sections and products were conducted using a validation algorithm. The results indicated that 0.96 mA/cm2 was the optimal impressed anodic current density in terms of a suitable polarized potential, uniform corrosion, and a valid corrosion product among the evaluated conditions.

Biography:

I research about corrosion of metals, especially, carbon steel and aluminum alloys. I am currently attending Sungkyunkwan University's graduate school as a Ph. D student, and this is my 4th year.

Synthetic Anti-Cancer Polymer Therapeutics to Target Cancer Cell Membrane

Haruko Takahashi*

Graduate School of Integrated Sciences for Life, Hiroshima University, JAPAN

Abstract:

Most anticancer drugs inhibit growth of cancer cells by targeting systems that regulate biosynthesis, which is related to cellular biological activities. However, small population of them, such as cancer stem cells and dormant cancer cells, gains resistance against these drugs owing to their slow proliferation, making chemotherapy difficult.

We have been developing synthetic polymers that exhibit effective anticancer activity against such refractory cancer cells by targeting the cell membrane. Synthetic polymers with properly controlled cationic and hydrophobic balances accumulate predominantly in cancer cells compared to normal cells and cause cell death by disrupting their cell membranes. Since

this mechanism is independent of cell proliferation, they can exhibit comparable anticancer activity even against cells that are difficult to treat with conventional anticancer drugs. In this presentation, we will discuss the results of our recent studies.

Biography:

Haruko Takahashi received her Ph.D. degree from the Tokyo Medical and Dental University, Japan in 2012. During 2012 to 2015, she was a postdoctoral researcher at University of Michigan followed by a project appointed assistant professor at the University of Tokyo from 2015–2018. From 2018, she is now an assistant professor in the Graduate School of Integrated Sciences for Life, Hiroshima University, Japan. Her research focuses on the design of biologically functional materials to treat cancer diseases, smart biosystems to model the 3D cancer tissue structures and characteristics, and their biomedical applications.

Novel Material Design to Prepare High-Performance Poly(Lactic Acid)

Masayuki Yamaguchi*

Japan Advanced Institute of Science and Technology, Japan

Abstract

Poly(lactic acid) (PLA) is known to show slow crystallization rate, weak melt elasticity in a molten state, and poor mechanical toughness in a solid state. In this presentation, various methods to solve these disadvantages are introduced. For example, a thin film with high impact strength is obtained by tubular-blown film processing by mixing a copolymer of ethylene and vinyl-acetate (EVA). The addition of EVA provides the strain-hardening behavior in elongational viscosity for a PLA melt, leading to improved bubble stability. The film with EVA shows a high level of impact strength. Cavitation in the dispersed EVA particles as well as shear yielding deformation of a continuous PLA phase are responsible for the mechanical toughness. Furthermore, a transparent film with a high level of crystallinity, which widens the service temperature greatly, is produced by adding a nucleating agent with a specific thermal history.

Biography:

After receiving a master degree from Kyoto university in 1989, he joined Tosoh corporation. In 1999, he received a doctor degree from Kyoto University. In 2005, he moved to Japan Advanced Institute of Science and Technology as an associate professor. In 2009, he was promoted to a full professor.

Modification of Mechanical Properties on Age-Hardenable Aluminum Alloys by Minor Elements

Kenji Matsuda

University of Toyama, Japan

Abstract

The effect of minor addition on clustering and precipitation in age hardenable aluminum alloys has been investigated by transmission electron microscopy (TEM). We have proposed it for several elements. For example, Cu addition enhances the formation of universal clusters

in age-hardenable Al-Cu-Mg, Al-Mg-Si, and Al-Zn-Mg alloys. Mechanical properties of Cu added Al-Zn-Mg alloys have been investigated by hardness measurement and tensile test. Their microstructures have also been observed by High Resolution Transmission Electron Microscopy (HRTEM) and Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM) techniques. An increasing amount of Zn + Mg caused higher hardness, strength, and lower elongation because of the increased number density of precipitates. The alloy containing the highest Cu content had fine precipitates of GPB-II zones or the second clusters, which we proposed as the universal cluster, in the precipitate free zones (PFZs) and the matrix, together with η'/η in the matrix from the early stage of aging. I will introduce those new topics in this talk.

Biography:

Matsuda is a professor and Deputy Dean of Faculty of Sustainable Design in the University of Toyama, Japan. He has also established the Center for Advanced Materials Research for International Collaboration (CAMRIC) in 2015 in there and was the director until 2020. His research interest is the phase transformation of metals at nano-scale using HRTEM. He has published over 200 publications, and he has 10 Japanese patents for Al and Mg alloys containing composite materials. He is the Board of directors, Japan Institute of Metals, Japan Institute of Light Metals, Councilor, Japanese Society of Microscopy, and Executive Scientific Committee of THERMEC, and also the Chairman of Steering Committee of ICAA18.

Improvement of Fatigue Strength of Additive Manufactured Ti6Al4V by Cavitation Peening Using a Submerged Water Jet and a Pulse Laser

Hitoshi Soyama

Tohoku University, Japan

Abstract

Additive manufactured (AM) metallic materials are attractive materials, as topologically optimized shapes can be realized and it is produced from CAD/CAM data directly. However, fatigue strength of AM metals is very weak comparing with bulk metals, as the surface of AM metals is very rough due to un-melted particles [1]. Shot peening is one of common methods to enhance the fatigue strength. Unfortunately, shots cannot treat the valleys between un-melted particles.

A novel peening method using cavitation impacts, which normally cause severe erosion in hydraulic machineries, has been developed, and it is called “cavitation peening” [2]. A conventional cavitation peening, cavitation is generated by a submerged high-speed water jet [3]. Note that “cavitation peening” is different from “water jet peening” in which water column impacts are used. And also, submerged laser peening is a kind of cavitation peening, as bubble is developed after laser ablation and the impact of the bubble collapse is larger than that of laser ablation [2].

In the invited presentation, the mechanisms of cavitation peening using the water jet and the pulse laser will be introduced, and the improvement of fatigue strength of AM Ti6Al4V manufactured EBM and DMLS by cavitation peening is demonstrated comparing with shot peening.

This work was partly supported by JSPS KAKENHI Grant Number 18KK0103 and 20H02021.

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[2] H.Soyama, Journal of Materials Processing Technology, Vol. 269, (2019), pp. 65 – 78.

[3] H.Soyama, Applied Sciences, Vol. 10, No. 20 (2020), DOI:10.3390/app10207280

Biography:

Hitoshi Soyama has completed his PhD from Tohoku University, Japan. He has been working at Tohoku University since 1991, and he was promoted to a professor at 2003. He was awarded as a Fellow of American Society of Mechanical Engineers ASME, and he is now president of Japanese Society for Multiphase Flow. He is known for his work in the fields of cavitation and its practical applications such as water treatment and mechanical surface treatment, i.e., cavitation peening. Although cavitation impacts causes severe damage in hydraulic machineries, his research utilized cavitation impacts for enhancement of fatigue properties of metallic materials.

Biobased Composites Materials from Waxes and Lignocellulosic Powders for Additive Manufacturing

Claire Mayer-Laigle* [1,2]
Alain Bourmaud[3]
Yi Chen[2]
Rob Whitton[2]
Maxime Barbier[2]
Johnny Beaugrand[3]
Benedicte Bakan[3]
Alan Dickson[2]
Marie-Joo Le Guen[2]

[1]IATE, Université de Montpellier, INRAE, Institut Agro-Montpellier SupAgro, 34060 Montpellier, France

[2]Scion, Rotorua, New Zealand

[3]Université De Bretagne-Sud, IRDL, CNRS, UMR 6027, BP 92116, 56321, Lorient Cedex, France

[4]Biopolymères Intéractions Assemblages (BIA), INRAE, Rue De La Géraudière, F-44316 Nantes, France

Abstract

Additive manufacturing (AM) is a way to rethink the design of new and functional objects by minimizing the quantity of material used compared to subtractive techniques. The AM application of biobased materials, or their composites sourced from biomass feedstocks, is key to reducing the impact of the human activities on the environment and contributing to a societal shift towards a circular bioeconomy. However, such materials are not easily implementable in current AM technologies due to technological limitations related to these materials' behaviours and morphologies. In the case of composite materials as feedstocks, the structure of the polymeric matrix and the interaction matrix and filler needs to be understood before adapting to the AM processes. In this study, we explored the use of biobased composite materials from waxes and fine lignocellulosic powders by two AM technologies: Paste Printing (PP) and Selective Laser Sintering (SLS). The starting raw materials (beeswax, pine-wax and lignocellulosic powders from different feedstocks) were characterized to understand their influence in the different processes. Composite powders were developed using an emulsion process to produce particles suitable for SLS application. The rheological properties of the pastes and the flow properties of the composite powders with different formulations were

studied to optimize the processability of the materials in both AM technologies. Objects with contents up to 60 wt.% of lignocellulosic powders were successfully printed and their functional properties were compared. Our preliminary results address different process behaviors from the raw materials based on their chemical composition and their physical behavior.

Biography:

Claire Mayer-Laigle is a research engineer from the French National Research Institute for Agriculture, Food and Environment (INRAe). During the last 8 years, she managed an INRAe facility for the plant materials processing in Montpellier (France). She has been a visiting researcher to SCION research institute in Rotorua (NZ) in the framework of an European grant : The SMARTPOP Project (H2020 - MFSAIF , grant Number 893040) with the aim to develop new sustainable and functional materials from lignocellulosic powder using additive manufacturing technique.

Raman Investigation for Near-Infrared (NIR) Reflective Black Pigments Based on Ca2(Mn,Ti)O4

Ryohei Oka*
Tomokatsu Hayakawa

Field of Advanced Ceramics, Department of Life Science and Applied Chemistry, Graduate School of Engineering, Nagoya Institute of Technology, Gokiso, Showa, Nagoya, 466-8555, Japan

Abstract

Ca_2MnO_4:Ti solid solutions were synthesized to investigate the detailed mechanism for the improvement of NIR reflectivity. Raman peaks at around 178, 290, 330, 463, 500, and 562 cm^{-1} were observed for all samples, while an additional peak was observed at around 780 cm^{-1} for the Ti^{4+}-doped samples, indicating that a silent A_{2g} mode was activated by doping Ti^{4+}, which mode was similar to a A_{1g} (breathing) mode found in B-site substituted simple perovskite structure. From the result that XRD did not exhibit any additional reflection, it could be concluded to be due to the presence of Ti–Ti correlation with a certain distance.

Biography

Ryohei Oka graduated doctoral degree at Tottori University in March 2021. He is Assistant Professor at Nagoya Institute of Technology from April 2021. He specializes in synthesis and characterization of inorganic pigments and optical materials containing transition metal ions.

Polymer Dielectric Composites with Stress-Sensitive Nanostructures for Capacitive Pressure Sensors

Gen-Wen Hsieh*
Shih-Rong Ling
Fan-Ting Hung
Pei-Hsiu Kao
Jian-Bin Liu

Institute of Lighting and Energy Photonics, College of Photonics, National Yang Ming Chiao Tung University, Tainan, Taiwan

Abstract

Touch sensing has found immense applications ranging from mobile communication and display to various wearable devices. Future artificial robots or amputees wearing tactile sensors could feel the sense of touch or the texture of the fingertip. Thus, a yearning for accurate, delicate touch sensing elements that could be implemented into healthcare and electronic skin has been envisaged. Toward this, flexible capacitive pressure sensors with high sensitivity and low detection limit, which can function in skin perception, fine touch, weak interaction, and gentle manipulation, are highly desired. Recently, elastomeric polymer, such as poly(dimethylsiloxane), has been regarded a promising material of choice as dielectric layer, because of its superior flexibility, elasticity, and biocompatibility. However, this elastomer is not able to produce enough deformation upon small pressure; after removal of pressure the relaxation time back to initial thickness is inactive. Although several methods of introducing microstructures/micropores into the dielectric layers have been discussed, they are generally complex and expensive.

Here, we demonstrate polymeric capacitive pressure sensors based on a novel composite dielectric film of poly(dimethylsiloxane) with zinc oxide tetrapod. These composite devices with an appropriate loading of tetrapods show remarkable sensing performance in capacitance change and sensitivity of 2.55 kPa−1 over that of pristine polymer sensors, enabling a minimum detectable pressure of only 1.0 Pa. Further, the operational stability, reliability and demonstration for monitoring physiological movements are also discussed. The proposed pressure sensors incorporating stress-sensitive zinc oxide nanostructures may open up a promising means for potential applications in ultrasensitive touch sensing, wearable device and electronic skin.

Construction of Morphotropic Phase Boundary of Multiferroic BiFeO3 Ceramics with Dynamical Electric and Magnetic Responses

Hua Ke[1*]
Liwei Zhang[1,2]
Hongjun Zhang[1]
Fangzhe Li[1]
Huijiadai Luo[1]
Lu Cao[1]
Dong Li[3]
Xiaoli Dong[3]
Guangtong Liu[3]
Yu Zhou[1]

[1]Harbin Institute of Technology, China

[2]Harbin University of Science and Technology, China

[3]Institute of Physics, Chinese Academy of Sciences, China

Abstract

ABO3 perovskite ceramics possess rich and complex phase transition sequences. From the perspective of crystal symmetry, morphotropic phase boundary (MPB) is introduced to obtain large ferroelectric polarization and magnetism for ABO3 multiferroic. Considering the remarkable strain (~14%) during the ferroelectric phase transition of bismuth ferrite (BiFeO3), one can achieve breakthroughs in ferroelectricity, piezoelectricity and large magnetoelectric coupling through reasonable design of composition and phases. Firstly, rare-earth (Er or Nd) substitution of A site is conducted to form Bi1-xRExFeO3 ceramics, constructing MPB structures at $0.1 \leq x \leq 0.2$ that promote polarization switching. The maximum remanent polarization 2Pr of the ceramics is ~58 μC/cm2, and the conductive mechanism of small polarons at the MPB is found. Secondly, magnetic domains are reversed by low voltages, and a permittivity change rate of 1.0%~1.4% is achieved at the magnetic field of 1T. When a large strain is introduced into BiFeO3 ceramics, it is found that the domain topographies heavily rely on the grain orientations. Finally, reversible rotation of the ferroelectric/magnetic order coupled with the local strain are observed by frequency-dependent electric/magnetic responses.

End of Day 04 Parallel session II

Oral Presentations

Interferometer-based Atomic Force Microscopy for quantitative nanoscale viscoelasticity

Shivprasad Patil*
ShatruhanSingh Rajput
Vikhyaat Ahlawat
Surya Pratap Deop a

Indian Institute of Science Education and Research, Pune India.

Abstract

Measurement of nanoscale viscoelasticity is of interest in single molecule limit along with other nanoscale systems wherein discrete molecular nature, as opposed to its continuum, dictates properties of materials more directly. After its advent, Atomic Force Microscope has been at the forefront in out attempts our measuring viscoelasticity at the level of single molecules . However, quantitative viscoelasticity, particularly in liquid environments is challenging due to possible artefacts arising out of hydrodynamics of the cantilever used to measure forces. In this talk, I will describe our attempts of separating the probe response from that of the molecule[1,2]. I will argue that interferometer-based AFM, wherein the displacements are directly measured is better suited for artefact free measurements , compared to the conventional deflection detection type scheme which measures cantilever bending[1], We have shown that a simple point-mass model depicting the cantilever can be used for data analysis if we measure displacements[3]. On the other hand, a detailed treatment with Euler-Bernoulli equation of bending of the beam may still produce artefacts in measurements performed with deflection detection scheme[1].

References:

1. S. S. Rajput , S. P. Deopa , J. Yadav, V. Ahlawat, S. Talele and S. Patil, Nanoscale viscoelasticity using Atomic Force Microscope in liquid environment, Nanotechnology, 32, 085103, (2021).
2. A. Ahlawat, SS Rajput, S. Patil. Elasticity of single flexible chains in good and poor solvent, Polymer, 230, 124031 (2021).
3. S. S. Rajput, S. P. Deopa, S. Kamerkar, V. J. Ajith and S. Patil , Validity of point-mass model in off-resonance dynamic Atomic Force Microscopy, Nanotechnology, 32, 405702 (2021).

Biography:

I am an experimental physicist. The main focus of my laboratory is to investigate how molecules respond to external mechanical perturbations at the boundary where continuum picture of matter breaks down. We develop novel experimental tools to measure diffusion through nano confined water and viscoelasticity of single macromolecules such as proteins, flexible polymers. A new interest in our lab is to develop novel methods to measure structured -ness of solvents.

PhD. University of Pune (2003)

Post-doc: Wayne State University (2003-05) and IMM, CSIC Madrid (2005-08)

Preparation of Si nano-wire array for various interesting application

Indrajit Mukhopadhyay[1*]
Suresh Vemuri[1]
Govind Gupta[2]
Harsh Chaliyawala[3]

[1]Pandit Deendayal Energy University, Gandhinagar, India

[2]NPL, New Delhi, India

[3]ICMPE, CNRS, Paris, France

Abstract

Si nanowire arrays have been in continuous focus of the researcher due to its high broadband absorption, high density and extra ordinary surface to volume ratio. These interesting properties demonstrate a very high potential for practical applications in advanced devices such as in transistors, photodetectors, light-emitting-diodes, solar cells and bio/chemical sensors. The application of Si-based photodetectors in light detection demonstrates low sensitivity in the ultraviolet and near infrared (NIR) regime, due to its low light absorption coefficient. Moreover, Si has an indirect band gap which results in low light sensitivity and it is mainly restricted in the visible to NIR light. Graphene on the other hand, exhibits an extremely high charge carrier mobility, a very broad spectral range of detection from ultraviolet to terahertz and quasi wavelength independent absorption, which is a result of its gapless band nature. In the present work, a Schottky heterojunction based IR photo-detector has been developed by placing few layer graphene on top of Si nano-wire array through a simple technique. The unique light trapping properties of Si nano-wire arrays, in combination of transparent conducting nature of graphene has been successfully utilised to fabricate an efficient NIR light trapping device. In another work, controlled acid vapor etching has been utilized in place of reactive ion etching to generate non-close pack assembly of Si nano-sphere. The non-close pack assembly has been used as template to fabricate Si nano-horn arrays for possible solar water splitting application.

Biography:

Indrajit Mukhopadhyay has been working as a Professor in the Dept. of Solar Energy, Pandit Deendayal Energy University, Gandhinagar, India. He received the prestigious CSIR Rural Technology Award 2008 and Vikram Sarabhai Award 2006 as a key team member for contribution in the field of chemical sciences while working at CSMCRI (CSIR), Bhavnagar, India. He received VIRA Distinguished Scientist in Solar Energy 2019. He was a visiting scientist at NIT, Japan during 2009. He published 150+ papers in international journal and has five US and one Indian patent in his credit.

Surface protective methods for increasing corrosion stability of dissimilar metal welds and high alloyed steels

Václav Bystrianský*[1]
Jaroslav Bystrianský[2]
Jan Macák[1]
David Dašek[1]
Petr Roztočil[1]
Aleš Návoj[3]

[1]Department of Power Engineering, UCT Prague, Prague, Czech Republic

[2]Faculty of Metallurgy and Materials Engineering, VŠB-TUO Ostrava, Ostrava, Czech Republic

[3]Department of Metallic materials and Corrosion Engineering, UCT Prague, Prague, Czech Republic

Abstract

Dissimilar metal welds are commonly used constructional solutions in most light-water reactors. Unfortunately, it may also be a source of operational problems due to the combination of two or more metals with different corrosion resistance. Our previous work has shown that corrosion stability of dissimilar metal welds can be also affected by the presence of impurities (S, P, C) reducing the corrosion resistance of austenitic steel, which can lead to atypical damage on the side of high-alloyed material

This self-contradictory phenomenon is presumed to be caused by segregation of impurities (S, P, C) from carbon steel on austenitic grain boundaries. For this reason, we've evaluated various methods of surface protection (thermal coatings, Ni layers) as a tool for successful protection of the weld surface in order to mitigate the effect of impurities and thus increase the service life of dissimilar metal welds.

Biography:

Václav Bystrianský is PhD student at UCT Prague, his research is focused on degradation mechanisms of high-alloyed steels and welded joints in power engineering. His work often combines electrochemical methods together with SEM/EDS analysis.

Sericin based Gold nanoparticles: Synthesis, characterization and biological applications

Gitishree Das[1]
Su Jin Seo[2]
Han-Seung Shin[2]
Jayanta Kumar Patra[1]*

[1]Research Institute of Biotechnology & Medical Converged Science, Dongguk University-Seoul, Goyang-si, Republic of Korea

[2]Department of Food Science and Biotechnology, Dongguk University-Seoul, Goyang-si, Republic of Korea

Abstract

Sericin, a water soluble protein, is usually removed from silk in a process called degumming as a biological waste material. This silk protein has numerous applications in the field of pharmaceutical, biomedical, cosmetic and food industries. Considering the vast potential of the sericin based materials, in the current investigation, an attempt has been made to extract sericin from the silk cocoon, purify it and study its bio-potential in terms of gold nanoparticle

synthesis and applications. The sericin was extracted from the silk cocoon by the degumming method. The protein concentration of the extracted crude sericin sample was estimated by the standard Lowry's method using the bovine serum albumin as the reference standard. Linearity was obtained (R2 > 0.99), and the protein concentration of the crude sericin was found out to be 3.60 % (W/V). The purification of the crude protein was carried out by the dialysis process using a cellulose tubing dialysis membrane with a molecular weight cutoff of 12 kDa, followed by freezedrying. Further, gold nanoparticles was synthesized using sericin as the reducing agents. After synthesis, the sericin based gold nanoparticles were characterized using various characterization techniques such as UV-Vis spectroscopy, Transmission electron microscopy, energy-dispersive Xray spectroscopy, dynamic light scattering zeta potential and Fourier-transform infrared spectroscopy. After characterization, the synthesized NPs were studied for their bio-potentials in terms of their antibacterial effect against a series of Gram positive and Gram negative foodborne pathogenic bacteria, antioxidant and wound healing activities. Keywords: Gold nanoparticles, Silk cocoon; Sericin; antibacterial; antioxidant; wound healing Acknowledgment: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2020R1G1A1004667), the Republic of Korea.

Biography:

Jayanta Kumar Patra, Ph.D., is currently working as Assistant Professor at Dongguk University, Republic of Korea. His current research is focused on nanoparticle biosynthesis and their application in bio-medical and agricultural fields. Dr. Patra has published more than 150 papers in various national and international peer-reviewed journals, 16 books, 32 book chapters. He is also editing two book series on Nanotechnology and Biotechnology for Elsevier and Springer Nature publications. Besides, he is editorial board member of several International Journals. Besides, Dr. Patra is listed under World's Top 2% Scientists based on citation impact during the single calendar year 2020-2021.

Dynamic surface potential mapping for direct evaluation of charge transport ability from organic crystals

Wen-Shan Zhang[1*]
Rasmus R. Schröder[2]

W.S. Zhang & R. R. Schröder: Centre for Advanced Materials, Universität Heidelberg & Bioquant, Univeristy Hospital Heidelberg, D-69120 Heidelberg, Germany

Abstract

Realizing high performance organic (opto-)electronic devices is of great interest in both academia and industry. One of the key points to success is to achieve high charge-carrier mobility, which is commonly obtained from organic thin-film transistors built with the desired materials. The measured mobility is, however, not only dependent on the chemical and physical properties of the material itself, but also relies strongly on the device fabrication. Non-ideal thin-film morphology and device structure can lead to a significant variation of the experimental data. This is a large obstacle for researchers to understand the correct structure-performance relationship and to draw a guideline for further material design.

Hereby, we would like to skip the step of device fabrication and directly estimate the charge transport ability from organic crystals. Using the ultra-low voltage scanning electron

microscopy, we are able to record the in-situ generated dynamic surface potential. As a result of charge transport ability, the distribution map of the dynamic surface potential on the semiconductor vary with beam energy, beam current, dwell time, pixel size etc., which allow us to assign the charge-carrier mobility within an order of magnitude. This method can be used for direct evaluation of the potential of newly synthesized materials for their use in organic electronics.

Biography:

Wen-Shan Zhang has studied Chemistry in Tsinghua University, P. R. China, and received her BSc degree in 2003. She moved to Germany and obtained MSc and PhD degree from University Ulm. She was then a postdoc in Eindhoven University of Technology, the Netherlands. Since 2017 she joined the Centre for Advanced Material, University Heidelberg, Germany. Her research interests mainly focus on synthesis, device fabrication and characterization of organic semiconductors.

Developing Emerging Inorganic Chalcogenides for Next Generation, Earth Abundant Photovoltaics

Nicolae Spalatu*
Robert Krautman
Jaan Hiie
Malle Krunks
Ilona Oja Acik

Tallinn University of Technology, Department of Materials and Environmental Technology, Ehitajate tee 5, 19086 Tallinn, Estonia.

Abstract

Development of new photovoltaic (PV) technologies based on novel green materials with higher efficiency and lower cost options could create a new industry with independent supply chains, foster IoT market diversification, and attenuate market volatility. Sb-chalcogenide compounds have recently gained increasing attention as defect tolerant, non-toxic and highly stable materials for earth abundant thin film polycrystalline PV technology. Despite of their recent addition to the thin film device canon, efficiency values of these materials have climbed rapidly and are now approaching 10%. Yet despite of this rapid progress, there is still headroom to increase performance significantly by addressing fundamental material challenges. This presentation will review the most relevant progress achieved for Sb-chalcogenides PV, with the emphasis on key processing strategies to optimize absorber material properties (doping and alloying), understanding of buried interfaces and push the boundaries of understanding and performance. Based on the state-of-the art progress in performance of emerging Sb-chalcogenide PV materials, a roadmap of application variability (including semitransparent and tandem PV devices for BIPV, PIPV and IoT markets) will be presented.

From an aluminum hazardous waste to nanomaterials for CO2 storage and valorization

Antonio Gil

INAMAT^2, Science Department, Los Acebos Building, Public University of Navarra, Campus of Arrosadia, 31006-Pamplona, Spain

Abstract

The work considers new applications of hazardous wastes generated during secondary aluminum melting processes. The composition of the saline slags is very heterogeneous including fractions of non-metallic products (various oxides), metallic aluminum and flux brines that restrains its application. Partially, saline slags have been recovered producing new liquid and solid wastes requiring further recycling or disposing in landfills. The present study considers saline slags as alternative aluminum source for the synthesis of nanomaterials (hydrotalcites, zeolites and hexaaluminates) for their further application as adsorbents and catalysts in the storage and valorization of CO2 by dry reforming of methane.

Biography:

Antonio Gil (Full Professor of Chemical Engineering, Universidad Pública de Navarra, Spain): Professor Gil earned his BS and MS in Chemistry at University of Basque Country (San Sebastián), and his PhD in Chemical Engineering at University of Basque Country (San Sebastián). He did postdoctoral research at the Université catholique de Louvain (Belgium) working on Spillover and Mobility of Species on Catalyst Surfaces. The research interests of Professor Gil can be summarized as: Evaluation of the porous and surface properties of solids. Pillared clays. Gas adsorption. Energy and CO2 storage. Pollutants adsorption. Environmental technologies. Preparation, characterization and catalytic performance of metal supported nanocatalysts. Industrial waste valorization.

Energy storage in super-activated carbon from agrifood wastes

Chiara Milanese,[1*]
Ilaria Frosia,[1,2]
Alessandro Girella,[1]
Simone Puoti,[1]
Vittorio Berbenni,[1]
Giacomo Magnani,[3]
Daniele Pontiroli,[3]
Mauro Riccò,[3]
Adele Papetti[2]

[1] Pavia Hydrogen Lab, C.S.G.I. & Chemistry Department, Università di Pavia, Italy

[2] Pavia FoodLab, Drug Science Department, Università di Pavia, Italy

[3] Nanocarbon Laboratory, DSMFI, Università di Parma, Italy

Abstract

Recently biochar, the carbon side-product in the pyrolysis/gasification of residual waste biomasses, started to receive a widespread attention in the field of energy-storage, thanks to its hierarchical porous structure inherited from biomass precursors, its excellent chemical and electrochemical stability, high conductivity, high surface area and inexpensiveness. In particular, biochar converted to activated carbon (SSA > 1000m2/g) through a chemical

treatment with KOH appears to be a new cost-effective and environmentally-friendly carbon material with great application prospect in the field of energy-storage. We report here on the preparation of novel hierarchically-porous super-activated carbon materials originating from biochar derived by the pyrolysis of agrifood wastes such as rice bran and husk, and melon and pumpkin peels. The chemical activation process proved to be efficient to remove the majority of impurities other than carbon, stabilizing highly porous hierarchical structures with local graphene-like morphology. The porous compounds obtained by rice bran and husk mixtures demonstrated to behave as excellent electrode materials for high-performance symmetric supercapacitors (SCs), reaching interestingly high specific capacitance. On the contrary, the materials obtained by rice bran or the vegetable peels, having specific surface area up to 3000 m2/g, show a very good hydrogen storage ability, adsorbing up to 4.5 wt % of hydrogen in around 20 seconds at 77K and around 1.5 wt% at room temperature. Work is in progress to optimize the pyrolysis and activation conditions and to improve the performance of the materials by decoration with transition metals.

Biography:

Chiara Milanese is associate Professor at the Physical Chemistry Section of the Chemistry Department – Pavia University, where she is the scientific coordinator of the Pavia Hydrogen Laboratory. Her main research activities regard the preparation and characterization of innovative materials for solid state hydrogen storage and energy storage and topic linked to circular economy. She is Italian expert of the task 40 "Energy storage and conversion based on hydrogen" activated by IEA and member of the International Hydrogen Carrier Alliance. She is author of more than 215 papers on materials science topics on high impact factor journals (h index 33).

Ceria-titania photoactive nanosystems for energy applications

Elisa Moretti[1*]
M. Gilzad Kohan[2]
A. Vomiero[1,2]
A. Infantes Molina[3]

[1]Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia, Italy

[2]Division of Materials Science, Department of Engineering Sciences and Mathematics, Luleå University-of Technology, 97187 Luleå, Sweden

[3]Department of Inorganic Chemistry, Crystallography and Mineralogy, University of Málaga, Campus de Teatinos, E 29071 Málaga, Spain.

Abstract

Nowadays, one of the main technological challenges that we are facing is the ability to provide a sustainable supply of clean energy and, among all renewable sources, solar energy displays the greatest potential.

Titania based systems are the most widely studied and applied photocatalysts. A growing interest has recently emerged on photoenergy applications of ceria, since its experimental band gap is very close to that of TiO2, with a decreased recombination rate of electron-hole pairs. Recently, the development of novel synthetic strategies has led to the preparation of nanostructured materials displaying unique properties compared to the bulk counterpart

systems, with controlled and tunable morphologies able to enhance the activity and selectivity of a catalytic process.

This talk will focus on the importance of tuning the morphological features of a catalyst as a strategy to improve the catalytic activity, focusing on how rationally designing ceria-based materials can lead to morphologies and micro/nanostructures suitable to enhance the catalytic performance. The talk will discuss some energy applications that can be addressed by ceria-titania nanosystems, highlighting their structure-reactivity relationship. Photocatalytic hydrogen production and purification will be presented as successful case history.

Biography:

Elisa Moretti is an Associate Professor of Inorganic Chemistry at the Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice (Italy). After receiving a PhD Degree in Chemistry (2005) at the Ca' Foscari University, she moved to the University of Malaga (Spain) for a post-doctoral experience. She is leading a multidisciplinary group focusing on the development of advanced 0-3D nanostructured inorganic materials for energy and environmental applications, including photocatalysis (on board H2 purification by CO preferential thermal/photo-oxidation, H2 production through water splitting, dyes and drugs photodegradation for water remediation).

High performance thermal insulations for temperatures above 1500 °C

Gudrun Reichenauer[1*]
Matthias Wiener[1]
Thomas Kirschbaum[2]
Martin Kucher[2]
Jürgen Hennicke[3]

[1]ZAE Bayern, Germany

[2]SGL Carbon GmbH, Germany

[3]FCT Systeme GmbH, Germany

Abstract

High temperature processes that are performed under non-oxidizing atmosphere in industrial applications well above 1000 °C, such as graphitization, synthesis of carbide or crystalline Si, are highly energy demanding. Thus, energy consumption in these processes can only significantly be reduced with thermal insulations possessing a largely improved performance. State of the art carbon based thermal insulations are based on graphitized carbon fibers panels. Due to the micron sized voids in between the fibers, these materials all show a strong increase in the thermal conductivity above 1000 °C indicating dominant radiative heat transfer. To suppress this heat transport path, we developped sol-gel based carbons (xerogels) with pores well below 1µm. Mechanical reinforcement for processing and handling was provided by fibers embedded in the xerogel. The synthesis was designed such that the manufacturing process can be up scaled to provide insulation panels with a thickness of up to 40 mm via convectional drying of the gel. The resulting panels are machinable and allow lamination e.g. with a graphite foil where needed. Comparing the thermal conductivity of the newly developed composite to a state of the art commercial high temperature insulation panel (MFA by SGL Carbon), reveals the significant reduction of the thermal conductivity of up

to a factor of 2 in the reange between 800 and 2200 °C. Evaluation of the novel insulation in a demonstrator furnace up to temperatures of 2200 °C shows that up to 30 % energy can be preserved under typical application conditions.

Biography:

Gudrun Reichenauer is head of the nanomaterials group at ZAE Bayern, Würzburg, Germany, since 2000. After her PhD in physics at Würzburg University, she pursued her career as a research associate at the Bavarian Center for Applied Energy Research, Würzburg University (1993-1998) and finally at Princeton University and at the Princeton Institute for the Science and Technology of Materials (USA, 1999-2000). Her scientific interests are focusing on the use of nanoeffects and the synthesis of scalable nanomaterials for applications in energy technology, as well as the development of new methods for rapid and artifact-free characterization of nanoporous materials.

Catalytic nanomaterials coupled with microwaves: good or bad?

Maela Manzoli[1*]
Silvia Tabasso[2]
Emanuela Calcio Gaudino[2]
Giorgio Grillo[2]
Fabio Bucciol[2]
Federica Menegazzo[3]
Michela Signoretto[3]
Giancarlo Cravotto[2]

[1]Drug Science and Technology Department, University of Turin and NIS - Centre for Nanostructured Interfaces and Surfaces, Torino, Italy.

[2]Department of Chemistry, University of Turin,Torino, Italy.

[3]CATMAT Lab, Department of Molecular Sciences and Nanosystems, Ca' Foscari University Venice and INSTM Consortium RU Ve, Venezia Mestre, Italy.

Abstract

According to the UN Sustainable Development Goals, the use of heterogeneous catalysis coupled with microwaves (MW) paves the way to industrial process intensification. However, the effects resulting from the interaction among the catalytic nanomaterials and MW are still not fully explored. To establish synergies between nanomaterials and MW, some case studies taken from the chemical-pharmaceutical field and waste biomass valorization are considered. The semi-hydrogenation of 2-butyne-1,4-diol to (Z)-2-butene-1,4-diol (BeD) is firstly described. BeD is an intermediate in the production of vitamin B6, insecticides and fungicides, as well as in the paper, textile and resin industries. Secondly, levulinic acid hydrogenation to 1,4-pentanediol (1,4-PDO) over gold-ased nanomaterials is illustrated. 1,4-PDO can be employed as monomer to produce polyesters, but also for the synthesis of organic solvents and medicines. Finally, cellulose conversion to 5-hydroxymethylfurfural (5-HMF) is discussed. 5-HMF can be catalytically oxidized to 2,5 furandicarboxylic acid, a possible alternative for terephthalic acid for plastic production.

Biography:

Maela Manzoli received the Ph.D in Chemistry in 2001. Her skills are in the study of surface properties of nanostructured catalysts as well as in their textural, morphological and structural characterisation before and after reaction to establish structure-activity relationships. She is currently associate Professor of Industrial Chemistry at the Department of Drug Science and Technology, University of Turin, where she started the development of new catalytic processes assisted by MW, US or mechanochemistry, with particular interest for biomass valorisation in both batch and flow reactors. She is author of >140 peer-reviewed papers and 3 book chapters (H-index: 42).

New materials used in the construction of all solid state ion-selective electrodes.

Cecylia Wardak[1*]
Karolina Pietrzak[1]
Szymon Malinowski[2]

[1]Maria Curie-Sklodowska University in Lublin, Poland

[2]Lublin University of Technology, Poland

Abstract

Thanks to their numerous technical advantages (easy operation of the equipment, speed of analysis, cheap apparatus, no need for special preparation of liquid samples) and analytical ones (very good selectivity, low detection limits) potentiometric methods are still very popular. The most popular sensors used in potentiometric methods are ion-selective electrodes (ISEs). Among the various design variants, ion-selective electrodes without an internal electrolyte solution are especially useful. Elimination of internal solution in all solid state ISEs was associated with deterioration in the stability and reversibility of the electrode potential as a result of the direct connection of two materials with different conductivity, notably the substrate electrode (electronic conductivity) and the ion-selective membrane (ionic conductivity), thus blocking the flow of charge at the interface. In order to obtain a satisfactory potential stability, at the same time with no internal solution, various additional material were used including conductive polymers, metal nanoparticles, carbon-based nanomaterials and others. In this study use of new composite materials in the construction of solid state ISEs were presented. Composite materials were obtained on the basis of multiwalled carbon nanotubes and other materials such as ionic liquids, CuO nanoparticles and conducting polymers. The basic analytical and electric parameters of the constructed sensors were examined in order to investigate the influence of modification on their performance. In addition, research was conducted to investigate the influence of variable conditions on the proper operation of the sensors (the effect of changes in solution pH and redox potential , the presence of light and oxygen) were carried out.

Biography:

Cecylia Wardak received the her Ph.D. degree in analytical chemistry in 2004 and her DSc degree in analytical chemistry and electrochemistry in 2015 from Maria Curie Sklodowska University (MCSU), Lublin, Poland. Since then she has been working as associate professor in the Department of Analytical Chemistry of Maria Curie-Sklodowska University. She is an active COST member. Her main scientific interests are research, development, and analytical applications of electrochemical sensors and biosensors. Her latest research focused on the use of nanomaterials and composite materials in the construction of ion-selective electrodes. She has published over 70 peer-reviewed papers.

Organosilica nanoparticles for nanomedicine: colloidal stability and degradability

Xavier Cattoën[1*]
Shridevi Shenoi Perdoor[1]
Jonas Croissant[2]
Michel Wong Chi Man[2]
Jean-Olivier Durand[2]
Magali Gary-Bobo[3]
Fabien Dubois[1]
Alain Ibanez[1]

[1]Univ. Grenoble Alpes, CNRS, Institut Néel, FRANCE

[2]Univ Montpellier, CNRS, ENSCM, Institut Charles Gerhardt Montpellier, France

[3]Univ Montpellier, CNRS, ENSCM, Institut des Biomolécules Max Mousseron, FRANCE

Abstract

Silica-based nanoparticles are widely investigated for nanomedicine, owing to their rigidity, biocompatibility, ease of preparation and possible functionalization. Including large amounts of organic groups within the inorganic matrix may strongly enhance the performance. The preparation of silica-coated organic nanocrystals will be described, which can be used for bioimaging in vitro and in vivo under two-photon excitation with a very high brightness. [1] We will then investigate methods to produce organosilica nanoparticles including large amounts of organic groups in order to provide increased degradability and drug loading. [2,3]

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Biography:

Cattoën obtained his PhD in molecular chemistry from the University of Toulouse, France, in 2004 under D Bourissou and G Bertrand. After three years of Post-Doc with MA Pericàs at ICIQ Tarragona, Spain, he was appointed CNRS researcher in Montpellier in 2007. He developed organosilica materials for catalysis, photonics and nanomedicine in close collaboration with M Wong Chi Man. In 2013, he moved to the Institut Néel in Grenoble where he is currently working on organosilica nanoparticles for biophotonics and drug delivery.

Experimental and Numerical Investigations of Auxetic Behavior and Topology Optimization for Additively Manufactured Polymers

Yanling Schneider[1]
A. Grebhardt[2]
V. Guski[1]
S. Schmauder[1]
Ch. Bonten[2]

[1]Institute for Materials Testing, Materials Science and Strength of Materials (IMWF), University of Stuttgart, Pfaffenwaldring 32, D-70569 Stuttgart, Germany

[2]Institut für Kunststofftechnik, University of Stuttgart, Pfaffenwaldring 32, D-70569 Stuttgart, Germany

Abstract

This work aims to achieve robust process parameters and investigate the auxetic behavior of designed and optimized inverse honeycomb structures. Typically, auxetic materials offer several new applications related to crash and safety. The selected materials are biodegradable polylactic acid (PLA), and polybutylene adipate terephthalate (PBAT) manufactured additively by fused filament fabrication modeling (FFF). Experimentally, specimens produced by the injection-molding process are firstly studied to obtain some essential characteristics of the tensile deformation behavior. The auxetic structure also experienced tensile deformations, including unloading-and-reloading hysteresis to provide simulation input data deducing the Mullins effect. Furthermore, the micro-computed tomography (μCT) combined with the digital image correlation (DIC) tests will provide more detailed insights into local auxetic deformation behavior. The manufacturing process is simulated by a thermo-mechanically coupled process based on the FE method (ABAQUS plug-in). The resulting structure and residual stresses are passed to the FE solver for mechanical simulations to determine the auxetic behavior. Another plug-in with consideration of self-contact will accomplish the topology optimization of auxetic structures. Results of the materials analysis illustrate that PBAT possesses extraordinary ductility and nearly linear stress increment after about 75% global strain. After hardening until about 2% global strain, the brittle PLA softens until failure at about 3% strain. Simulations on the auxetic behavior deliver high stress and strain values in regions near to vertexes of two walls in the structure. The comparison of the experimental and simulation results, e.g., the local stress, strain distribution, displacements, and the structural Poisson's ratio, provide a good agreement.

Biography:

The presenter works in the field of numerical investigations of material deformation behaviors, including topology optimization, for metals, composites, and polymers on different scales. Usually, such studies are coupled with experimental ones. She is also interested in the big-data-driven science applied in materials science.

Switching from Single to Simultaneous Free-Radical and Anionic Polymerization with Enamine-Based Organic Electron Donors

Julie Broggi[1*]
Yuxi Zhao[1]
Marion Rollet[1]
Laurence Charles[1]
Gabriel Canard[2]
Didier Gigmes[1]
Patrice Vanelle[1]

[1]Aix Marseille Univ, CNRS, Institut de Chimie Radicalaire (ICR), Marseille (France)

[2]Aix Marseille Univ, CNRS, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Marseille (France)

Abstract

Although most monomers can polymerize through different propagation pathways (cationic, radical, anionic, ...), rare are the polymerization initiating systems that can switch from one mode to another. Accordingly, the simultaneous initiation of different polymerization modes in a one-pot setup requires three-component systems mixing two types of activators (one as radical promoter and one as cationic or anionic promoter) with an additive.

Our project was thus to develop a single initiating system capable of simultaneous radical and anionic polymerizations of two monomers. In the wake of our recent organic electron donors (OED)-promoted anionic process, we now demonstrate that organic electron donors are also remarkable initiators for the radical polymerization of a large range of monomers. Our light-, metal- and peroxide-free strategy allows the preparation of a large variety of polymers. Introduction of a competing oxidant with a higher reduction potential than the monomer switches the former anionic propagation to a clean radical propagation process. Thereby making OED the first system able to initiate either independent or simultaneous radical or anionic polymerizations under simple, mild and safe conditions. The benefit of this dual-mode activator is highlighted in the synthesis of interpenetrating polymer networks through simultaneous initiation of radical and anionic propagation processes.

Biography:

Julie Broggi is Assistant Professor at the Faculty of Pharmacy, Aix Marseille university. Her research interests focus on the synthesis and reactivity of nitrogen-containing heterocycles used as organic electron donors. She designs air-stable precursors of these powerful reducers to improve their practicability. She also explores their reactivity in the reduction of uninvestigated species and for unprecedented applications including therapeutic or polymer chemistry.

Tannin based porous polymers – synthesis and characteristic of properties

Magdalena Sobiesiak[1*]
Pawel Parzymies[1]

Maria Curie-Sklodowska University Poland

Abstract

Tannins are a group of natural polyphenols. One of the representatives of hydrolyzable tannins (gallotannins) is tannic acid. This compound possesses interesting chemical properties, resulting from the presence of active hydroxyl groups which can be used in modification processes.

The presented studies describe the synthesis of tannin bases polymeric materials with the use of pristine or chemically modified tannic acid. Porous polymeric materials have been synthesized by the suspension method in two types of research systems. In the first one a mixture of components: pristine tannin (T), glycidyl methacrylate (GMA) and divinylbenzene (DVB) was polymerized. In the other, at first glycidyl methacrylate was chemically bound to the tannin and then the resulting product was copolymerized with divinylbenzene. The modification of tannin was a spontaneous reaction proceeding at room temperature. Its course was confirmed by FTIR and NMR spectroscopy analyses. Depending on the mechanism of the GMA epoxide ring opening reaction two products were obtained, which differed in color from each other. One was yellow and the other was brick red.

The conducted research proved that tannin can be used in the synthesis of porous polymers, both in the free state and as a chemically modified component. The obtained polymeric materials possessed different porosity and ability to absorb water and organic solvents. Their sorption properties were tested as uptake of phenolic compounds and non-steroidal anti-inflammatory drugs form aqueous solution.

Biography:

Magdalena Sobiesiak received a M. Sc. in Chemistry at the Maria Curie Sklodowska University in Lublin, where later obtained a degree ScD and habilitation in Chemical sciences. She is a research scientist and academic teacher at the Department of Polymer Chemistry in MSCU. Her work focuses on the synthesis and modification (physical and/or chemical) of porous polymers and carbons, based on components synthetic, natural or both, as well as characterization of the porous materials and their application in sorption and separation processes of organic compounds (mainly phenolic derivatives) and pharmaceuticals.

Bright red-emitting hetero-bimetallic complexes for efficient light-emitting electrochemical cells

Anna Bonfiglio
[a]Pei-Wan Hsiao
[b]Christophe Gourlaouen
[c]Vincent César
[d]Stéphane BelleminLaponnaz

[a]Chantal Daniel,c Federico Polo,e Hai-Ching Su,b and Matteo Mauroa a IPCMS, Université de Strasbourg & CNRS, Strasbourg (F)

[b]Institute of Lighting and Energy Photonics, National Chiao Tung University, Tainan 71150, Taiwan.

[c]Lab. Chimie Quantique, Institut de Chimie UMR7177 Université de Strasbourg, Strasbourg (F)

[d]LCC-CNRS UPR8241, Université de Toulouse, CNRS, Toulouse, France

[e]Dept. of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Venezia (Italy)

Abstract

Phosphorescent complexes are under current intense investigation in materials science due to their outstanding photophysical and redox properties and their application as triplet emitters in phosphorescent light-emitting devices, such as OLEDs and LECs. Nevertheless, achieving bright emission in the red and near infrared (NIR) region is highly challenging due to energy gap law consideration. Hence, efficient red/NIR light-emitting devices are still scarce, inspite of their importance in fields such as biomedical and display technology. Herein, our most recent results in the field will be presented including a novel class of phosphorescent cationic heterobimetallic IrIII/MI complexes, where MI = CuI and AuI where the two metal centers are connected by the hybrid bridging 1,3-dimesityl-5-acetylimidazol-2-ylidene-4-olate (IMesAcac) ligand that combines both a chelating acetylacetonato-like and a monodentate N-heterocyclic carbene site coordinated onto an IrIII and a MI center, respectively. These cationic bimetallic species display vibrant red emission with up to two-fold increase of the photoluminescence quantum yield and radiative rate constant compared to the corresponding mononuclear benchmarks, and achieve record PLQY up to 77%. This finding is associated to the smaller energy gap between the metal-to-ligand charge transfer (1,3MLCT) and the ligand center (3 LC) manifolds that mix via spin-orbit coupling and configurational interaction. Finally, their successful application as electroluminescent materials in light-emitting electrochemical cells (LECs) will be presented, which show external quantum efficiency up to 6%. In spite of the simple single-layer solution-processed device architecture, these values are the highest one for bimetallic emitters to date and amongst the highest for red LECs.

Biography:

Matteo Mauro obtained his MSc and PhD (2009) degrees in Chemical Sciences from the University of Milan. After an Alexander von Humboldt postdoctoral fellowship at the WWU Münster (Germany, he was appointed as an Assistant Professor at the University of Strasbourg, France (2012). Since 2018, he is an independent group leader at the IPCMS in Strasbourg. He has been awarded with the ENI Award (2010) and the 2019 Young Researcher prize of the Coordination Chemistry Division of the French Chemical Society. He serves as an Early-Career Advisory Board member for ChemPhotoChem. His research deals with i) luminescent compounds for light-emitting devices; ii) shape-morphing materials driven by light.

Chitosan-based hydrogels: a family of materials for Tissue Engineering applications

Alessio Bucciarelli[1*]
Antonella Stanzione[1,2]
Giuseppe Gigli[1,2]
Lorenzo Moroni[1,2]
Alessandro Polini[1]
Francesca Gervaso[1]

[1]CNR NANOTEC – Institute of Nanotechnology, National Council of Research, Italy

[2]Dipartimento di Matematica e Fisica E. de Giorgi, Università Del Salento, Italy

[3]MERLN Institute for Technology-Inspired Regenerative Medicine, Maastricht University, Netherlands

Abstract

Chitosan is a polysaccharide derived from chitin, the second most abundant polysaccharide in the world, after cellulose. Due to its remarkable properties, it has a wide applicability in tissue engineering, and in particular for the development of bioinks able to support 3D cell culturing. In this context, we developed a family of chitosan-based stimuli-responsive hydrogels with a Young modulus that ranges from few kPa to 30 kPa, suitable to match the Young modulus of different biological tissues. This family is composed by thermo-crosslinkable and composite interpenetrated network materials (made of chitosan only or in combination with Pectin and GelMa). As further addition to this plethora of materials, we recently developed a photo-crosslinkable methacrylated chitosan (CS-MA) that, being water soluble at physiological pH conditions, is cell encapsulation-ready. CS-MA was produced by chemical modification, grafting vinyl groups to the chitosan chain. This allowed the radical polymerization triggered by the exposure to UV light. Tuning the hydrogel composition (in terms of CS-MA and photoinitiator concentrations) and process parameters (in terms of UV-exposure time and adsorbed energy) impacted the mechanical response, microstructure, and degradation. As a consequence, also the biological properties were modified. By the use of statistical methods (Design of Experiment and Response Surface Method) we were able to relate by empirical equations the composition of the hydrogel and the process parameter to the outcoming property of the gel. As a result, it was possible to accurately control the material properties and tune them not by trial-and-error but resolving a system of equations.

Biography:

Alessio Bucciarelli background is in the processing of natural polymers, mainly silk fibroin, silk sericin, keratin, and chitosan, all promising materials for tissue engineering. The innovative activity of the application of statistical methods on optimization problems in Tissue Engineering allowed him to publish his works in important international journals (Advanced Functional Material, Advanced Material Interface, ACS Applied Materials and Interfaces). He has several active collaborations with national and international institutions (Jeonbuk Univeristy, TUFTS University, Rizzoli institute, Trento University, Bruno Kessler Foundation) where he performs data analysis to optimize processes in biomaterial fabrication.

Thermosensitive polymeric hydrogels and organogels: from supramolecular structure to new drug-delivery systems for inflammatory diseases treatment

Daniele Ribeiro de Araujo

Drugs and Bioactives Delivery Systems Research Group (SISLIBIO). Human and Natural Sciences Center, Federal University of ABC. Av. dos Estados 5001, Bl A, T 3, Lab 503-3, Bangu. Santo André, SP, Brazil. CEP 090210-580.

Abstract

Poloxamers (PLs) copolymers are composed of polyethylene oxide (PEO) and polypropylene oxide (PPO) units, able to self-assemble in micelles due to the PPO dehydration groups and micellar aggregation, forming hydrogels at a critical gelation temperature. Additionally, the incorporation of different components (drugs, surfactants, oils, polymers, nanoparticles, organic solvents, solubilizers) into PL-based hydrogels has driven investigations regarding to their influence on supramolecular structure and prediction of biopharmaceutical properties. Our research group has studied the development and pharmacological evaluation of PL-based hydrogels and organogels in the light of their structural organization and the influence on drug release/permeation performance looking forward the treatment of inflammatory diseases such as ulcerative colitis, osteoarthritis and atopic dermatitis. More recently, we have also devoted to the study of PL-based organogels, associating different oil phases (lecithin, lanolin), as well as the association of PL with natural polymers (such as hyaluronic acid, cellulose derivatives) or other nanocarries (such as polymeric/lipid nanoparticles) considering them as new delivery systems strategies modulated by their temperatures relative to micellization/gellation and rheological properties. The most pronounced structural changes were observed on drug release and permeation/release profiles, since slower constants were obtained according to the hydrophobic PL or polymeric nanoparticles insertion, because of their different phase organization transitions. In addition, the incorporation of different oil phases enhanced the drug permeation across artificial and biological membrane skin-models, point out the application of both systems as new drug delivery systems. Funding: (CNPq # 309207/2016-9, 402838/2016-5, 307718/2019-0; FAPESP 2019/20303-4).

Biography:

Pharmacy Bachelor (Federal University of Maranhão, Brazil), Master and PhD in Biochemistry (State University of Campinas, São Paulo, Brazil). Associate Professor in Pharmacology (Federal University of ABC, Brazil). Research fields in Nanobiotechnology on development of Poloxamer-based systems such as micelles, hydrogels, organogels. Structural and physico-chemical evaluation of epidermis for skin-delivery design. Design and development of drug-delivery systems for the treatment of inflammatory diseases (osteoarthritis, rheumatoid arthritis, atopic dermatitis). 98 articles; 11 book chapters, 4 editions, 8 patents. 2800 citations and H-index = 33 (GoogleScholar); 1586 citations and H-index= 26 (Scopus). Editorial board: Pharmaceutics, Future Pharmacology Biomed Res Int and Frontiers in Pharmacology.

Tuning Functional Carbon Nanodots for Regulating Cellular Oxidative Stress

Jianjun Wei*
Mahsa Azami
Zuowei Ji
Durga M. Arvapalli

The Department of Nanoscience, Joint School of Nanoscience and Nanoengineering (JSNN), University of North Carolina at Greensboro, Greensboro, NC 27401, US

Abstract

Carbon nanodots (CNDs) have attracted tremendous attention since their discovery in 2004 because of their superior water solubility, biocompatibility, photoluminescence, and opto-electronic properties. As such, CNDs have been reported potentially for broad applications in biomedicine, bioimaging, biosensor, and drug delivery systems. It becomes essential to investigate the activities of CNDs in biological systems by tuning the functionalities of CNDs including compositions, surface groups and charges, etc. We report some recent findings of how the structures and functions of CNDs influence the cellular uptake, subcellular location and oxidative stress effect in terms of the regulating the reactive oxygen species (ROS) in living cells. We designed and synthesized a series of CNDs from selected precursor molecules by doping different elements thus forming distinctive functional groups in the CNDs. The doped CNDs demonstrate strong antioxidant capacity by scavenging free radicals in physicochemical testing, however they may show opposite effect in two cell lines, EA.hy926 and A549 cells, associated to the dopants. For instance, the N-doped CNDs offer high biocompatibility as an antioxidant by scavenging ROS in the cells, while the N,S-CNDs present strong prooxidant effect by stimulating higher level ROS. These results provide evidence that more systematic research on tuning structure-functions of the CNDs may render the regulation of the oxidative stress in living cells and beyond.

Biography:

Jianjun Wei is Professor of Nanoscience at the Joint school of Nanoscience and Nanoengineering (JSNN), the University of North Carolina at Greensboro (UNCG). Dr. Wei joined the JSNN/UNCG in 2013. Dr. Wei's research at JSNN has been supported by grants from NSF, NIH, NCBC, DOD and NC state funding. Prior to joining JSNN, he had worked in CFD Research Corporation in Huntsville, AL, and led as a Principal Scientist for several BAA, SBIR/STTR Phase I, II, and III projects, primarily through NIH, NASA and DOD grants. He obtained his Ph.D. in chemistry in 2004 at University of Pittsburgh.

Novel carrier transport through metal contact of 2D semiconductors decorated by monolayer boron nitride

Huamin Li*

University at Buffalo, The State University of New York

Abstract

2D semiconductors such as monolayer molybdenum disulfide (MoS2) are promising material candidates for next-generation nanoelectronics. However, there are fundamental challenges related to their metal–semiconductor (MS) contacts, which limit the performance potential for practical device applications. In our recent work, 2D monolayer hexagonal boron nitride

(h-BN) is exploited as an ultrathin decorating layer to form a metal–insulator–semiconductor (MIS) contact, and an innovative device architecture is designed as a platform to reveal a novel diode-like selective enhancement of the carrier transport through the MIS contact. The contact resistance is significantly reduced when the electrons are transported from the semiconductor to the metal, but is barely affected when the electrons are transported oppositely. A concept of carrier collection barrier is proposed to interpret this intriguing phenomenon as well as a negative Schottky barrier height obtained from temperature-dependent measurements, and the critical role of the collection barrier at the drain end is shown for the overall transistor performance.

Biography:

Huamin Li is an Assistant Professor in Department of Electrical Engineering, the University at Buffalo. He is an IEEE Senior Member and Editorial Board Member of IEEE Access and Nano Express. His expertise lies in 2D nanomaterials engineering and their nanoelectronic applications.

Irradiation and temperature-dependent diffusion in UMo for research reactor applications

Benjamin Beeler[1,2*]
Park Gyuchul[3]
Maria Okuniewski[3]
Yongfeng Zhang[4]
Shenyang Hu[5]
Zhi-Gang Mei[6]

[1]North Carolina State University, USA

[2]Idaho National Laboratory, USA

[3]Purdue University, USA

[4]University of Wisconsin-Madison, USA

[5]Pacific Northwest National Laboratory, USA

[6]Argonne National Laboratory, USA

Abstract

Under the United States High-Performance Research Reactor (HPRR) program, several research reactors are planned to undergo a conversion to U-Mo monolithic fuel. The accurate prediction of fuel evolution under irradiation requires the implementation of correct thermodynamic and kinetic properties into fuel performance modeling. One such property where there exists incomplete data is the diffusion of relevant species under irradiation. Fuel performance swelling predictions rely on an accurate representation of diffusion to determine the rate of fission gas swelling and local microstructural evolution. In this work, molecular dynamics simulations have been combined with cluster dynamics calculations to determine the intrinsic, radiation-enhanced, and radiation-driven diffusion of U, Mo, and Xe as a function of temperature and fission rate. This study completes the multi-component diffusional picture for the U-Mo system, providing necessary information for the study of fission gas swelling evolution.

Biography:

Beeler received his B.S., M.S., and Ph.D. degrees in Nuclear and Radiological Engineering from the Georgia Institute of Technology. He was a post-doctoral researcher jointly at the University of California, Davis and the University of California, Berkeley. Prior to joining the NC State faculty, he was a computational scientist in the Computational Microstructure Science group in the Fuels Modeling and Simulation department at Idaho National Laboratory. He is the current lead of the Microstructure Fuel Performance Modeling working group for the United Stated High-Performance Research Reactor program.

Cellulose-based Flexible Materials for Emerging Multifunctional Sensing

Anthony B. Dichiara[1*]
Sheila M. Goodman[1]
Heather G. Wise[1]
Dylan D. Edmundson[1]
Jae-Hyun Chung[2]

School of Environmental and Forest Sciences, University of Washington, Seattle, WA 98195, U.S.A.
Mechanical Engineering Department, University of Washington, Seattle, WA 98195, U.S.A.

Abstract

Papertronics is an attractive technology to meet the growing demands for naturally abundant, biocompatible, biodegradable, flexible, inexpensive, lightweight and highly miniaturizable sensory materials. In particular, grafting electrically conductive nanoparticles onto the surface of cellulose pulp fibers prior to sheet formation offers opportunities to manufacture papers with greater control over the percolated network of fillers constituting electric paths in the fibrous structure. Flexible papers whose electrical characteristics are responsive to various environmental stimuli, such as moisture or mechanical stress, are produced based on a scalable, aqueous-phase, dynamic web forming process. The interfacial interactions between the nanofillers and the cellulose components are thoroughly characterized. The multifunctional capacitive and resistive sensing performance of as-prepared materials are assessed in models simulating real world applications. This research has important implications for circularity and sustainability to enable the future bioelectronics and wearable devices.

Biography:

Anthony B. Dichiara is a Weyerhaeuser-Endowed Associate Professor of Bioresource Science & Engineering at the University of Washington, Seattle WA. His research encompasses every aspect related to the sustainable design and engineering of advanced materials, from the synthesis and characterization of innovative bio-sourced nanoparticles to their assembly, both in the laboratory and large-scale facilities, into multifunctional composites with exceptional performance in catalytic, environmental, and electronic applications. His research production includes over 50 peer-reviewed publications in higher impact journals, 5 journal covers, 1 book chapter, and 5 patents and disclosures with 2 being licensed for commercialization purposes.

Defect and Interface/Interphase Engineering in Electrode Materials for Metal Ion Batteries

Hui (Claire) Xiong

Boise State University, USA

Abstract

Rechargeable batteries are promising energy storage technologies to provide high energy and high power for applications such as electric vehicles and electrical grids. Recent studies have shown enhanced electrochemical charge storage in electrodes that contain intentional structural defects (e.g., vacancies and interstitials) or with tailored interfaces/interphases. In this talk, recent works in my group including engineering defects in electrode materials through ion irradiation, and operando electrochemical cycling, as well as interface engineering in composite electrodes and studies of solid electrolyte interphases for metal ion batteries (e.g., Li ion and Na ion batteries) will be discussed. Perspectives regarding new pathways to design and engineering defects and interfaces in electrode materials with enhanced energy/power for rechargeable batteries will be given.

Biography:

Hui (Claire) Xiong is an Associate Professor in the Micron School of Materials Science and Engineering at Boise State University. Dr. Xiong received her BE degree in Applied Chemistry, MS degree in Inorganic Chemistry from East China University of Science and Technology, and her Ph.D. in Electroanalytical Chemistry from the University of Pittsburgh in 2007. Dr. Xiong received NSF CAREER Award in 2015, has been a Scialog Fellow and the Fellow of the Center for Advanced Energy Studies. Her research focuses on design, development, and characterization of advanced energy materials for Li-ion, Na-ion batteries and beyond.

Shakedown Limits and Uses in Railroad Engineering

Nazmul Hasan

SNC-LAVALIN, 745 Thurlow Street, Vancouver, BC, Canada

Abstract

A Poisson's ratio of 0.3 has usually been used for all grades of steel to estimate the shakedown limits, however high strength steel, heat-treated pearlitic steel, work-hardened (strain-hardened) steel, and newly developed bainitic steel show better response to deformation than standard carbon steel and the characteristics of the particular steel is to be considered. Elastic and plastic shakedown limits were expressed in terms of the tensile and yield strength using the Von Mises yield criterion and Hertz contact theory. Hence, shakedown limits can be computed, and a diagram can be created for each specific steel. Therefore, different steels may be compared to facilitate selection of the appropriate grade of steel. In this study, the elastic and plastic shakedown limits were computed for three grades of American Railway Engineering and Maintenance-of-Way Association (AREMA) steel. Finally, AREMA high strength steel and DOBAIN steel were compared.

Biography:

Nazmul Hasan M Eng P Eng is a Principal Track Expert, SNC Lavalin Inc. since 2006. Hasan holds M. Eng. Degree (by research) from the University of Newcastle, Australia and B. Sc. in

Civil Engineering from Bangladesh University of Engineering and Technology (BUET), Dhaka. Hasan authored over two dozen of journal and peer reviewed conference e.g., JRC, ICTD papers on track design issues. He published papers in ASCE journals – Journal of Transportation Engineering, Parts A :Systems (JTEA), Journal of materials in Civil Engineering (JMCE), Practice Periodical on Structural Design and Construction (PPSDC); Journal of Rail and Rapid Transit (JRRT), UK. Hasan is a registered professional engineer with APEGBC, PEO in Canada and EA in Australia.

Friction Stir Welding and Self-Ion Irradiation Effects on Microstructure and Mechanical Properties Changes with on Oxide Dispersion Strengthened Steel MA956

E. Getto*
M. Johnson
M. Maughan
N. Nathan
J. McMahan
B. Baker
K. Knipling
S. Briggs
K. Hattar
M.J. Swenson

[1]United States Naval Academy, Annapolis, MD, USA

[2]University of Idaho, Moscow, ID, USA

[3]Naval Research Laboratory, Washington, DC, USA

[4]Sandia National Laboratories, Albuquerque, NM, USA * Email: getto@usna.edu, 410-293-6506

Abstract

The joining process for oxide dispersion strengthened (ODS) alloys remains a key challenge facing the nuclear community. The microstructure and mechanical properties were characterized in the base material and friction stir welded ODS MA956 irradiated with 5 MeV Fe++ ions from 400 to 500°C up to 25 dpa. Nanoindentation was performed to assess changes in hardness and yield stress, and the dispersed barrier hardening (DBH) model was applied to described results. A combination of scanning transmission electron microscopy (STEM) and atom probe tomography (APT) were used to assess evolution of the microstructure including dispersoids, network dislocations and dislocation loops, nanoclusters, and solid solution concentrations. Overall, softening was observed as a result of increased dose, which was exacerbated at 500°C. The formation and coarsening of new dispersoids was noted while nanoclusters tended to dissolve in the base material, and were not observed in the stir zone. Solute nanocluster evolution was identified as a primary driver of the changes in mechanical properties.

Biography:

Elizabeth Getto (née Beckett) received her B.S. in Nuclear Engineering from Purdue University, graduating with highest distinction, and her M.S. and Ph.D. in Nuclear Engineering from the University of Michigan. Throughout graduate school, she specialized in nuclear materials and radiation effects. Dr. Getto is currently an assistant professor at the United States Naval Academy in Annapolis, Maryland in the Mechanical Engineering Department. Her current collaborations include work with the University of Idaho and Naval Research Laboratory on prospective reactor materials and weldments and with Naval Surface Warfare Center (NSWC) Crane on radiation effects on additive manufacturing of polymers.

Advanced nanostructured microcantilever sensors for the detection of nerve agents

Guillaume Thomas[1*]
Laurent Schlur[1]
Geoffrey Gerer[1]
Thomas Cottineau[2]
Valérie Keller[2]
Denis Spitzer[1]

[1]Nanomatériaux pour les Systèmes Sous Sollicitations Extrêmes (NS3E), UMR 3208 ISL/CNRS/UNISTRA, French-German Research Institute of Saint-Louis, France

[2]Institut de Chimie et Procédés pour l'Energie, l'Environnement et la Santé (ICPEES), UMR 7515 CNRS/ Université de Strasbourg, 25 rue Becquerel, 67087 Strasbourg, France.

Abstract

Potential exposure to Chemical warfare agents (CWAs) and explosives from terrorist organizations or military groups is nowadays significant. The development of sensors with high selectivity and sensitivity becomes necessary to effectively protect civilian populations and army forces against these threats. To detect these molecules in vapor phase and at low concentration, we developed bio-inspired nanostructured and functionalized microcantilevers with optical or piezoresistive readout technique. One or both sides of the microcantilever surface can be nanostructured in order to enhance highly the surface area of the sensor, allowing a higher capture of molecules and thus improving the sensitivity. This strategy overcomes one of the principal limitations of microcantilever sensors, which is a low surface area of capture. Metallic oxides (TiO2, MnO2, CuO and Cu(OH)2) with different morphologies (nanotubes, nanorods and nanoflakes) showed high interactions with a conventional simulant of sarin (GB), the DiMethyl MethylPhosphonate (DMMP). Then, the surface of the microcantilevers was functionalized in order to improve the selectivity and sensitivity of the microcantilever by using bifunctional molecules. In addition, an analytical method to model the adsorption processes of low traces of CWAs in vapor-phase was applied and we observed that morphologies of nanostructures play an important role in the diffusion regimes of molecules during the adsorption. These strategies allowed to reach a limit of detection under ppm level.

Biography:

Since joining the French-German Research Institute of Saint-Louis (ISL), Guillaume has been involved with studies related to the nanostructuring and functionalization of microcantilevers for the detection of chemical warfare agents in vapor phase. Before joining ISL, Guillaume worked at the Commissariat à l'Energie Atomique (CEA) as postdoctoral researcher and conducted researches in the field of DNA origami-driven lithography for patterning of silicon surfaces.

Natural Self-Assembly of Metal Phosphate Nanotubes into One- and Two-Dimensional Nanoarchitectures for Electrocatalytic Applications

Yusuf Valentino Kaneti[1*]
Ni Luh Wulan Septiani[2]
Kresna Bondan Fathoni[2]
Yusuke Ide[3]
Brian Yuliarto[2,4]
Hermawan Kresno Dipojono[4]
Dmitri Golberg[6]
Yusuke Yamauchi[1,3]

1) Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Brisbane, QLD, 4072, Australia

2) Advanced Functional Materials Laboratory, Department of Engineering Physics, Institute of Technology Bandung (ITB), Bandung 40132, Indonesia

3) JST-ERATO Yamauchi Materials Space-Tectonics Project and International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

4) Research Center for Nanosciences and Nanotechnology (RCNN), Institute of Technology Bandung (ITB), Bandung 40132, Indonesia

5) International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

6) Centre for Materials Science and School of Chemistry and Physics, Faculty of Science, Queensland University of Technology, Brisbane, QLD 4000, Australia Email: v.kaneti@uq.edu.au

Abstract

Transition metal phosphates have attracted increasing interest for energy storage and conversion applications due to their layered structures and high electrochemical activities.1-3 Furthermore, the open-framework structures of metal phosphates consisting of large channels and cavities and their rich redox behavior can provide high ionic conductivity and good transport path for ions.4 In addition, the P−O covalent bonds present in metal phosphates are strong, which impart them with high chemical stability. Moreover, the oxyanion of pentavalent phosphorus can lead to a large variety of metal phosphate phases.5 This wide variety in valence states can lead to change in oxidation states during surface reactions, which in turn can enhance their electrical conductivity for electrocatalytic applications. This presentation will discuss the achievement of self-assembly of bimetallic nickel-cobalt (Ni-Co) phosphate (Ni-Co HPi) nanotubes into one- (1D) and two-dimensional (2D) sheet-like architectures using Ni-Co glycerate spheres as templates.6, 7 The unique self-assembly of these metal phosphate nanotubes into 1D/2D structure is promoted by the "wrap-peel-weave" mechanism. The electrocatalytic measurements reveal that the Ni-Co HPi sample with nanotubes-assembled sheet-like structure exhibits the highest activity and stability for oxygen evolution reaction (OER) with negligible current density attenuation of less than 2% after 15 h of continuous cycling. Post-cycling XPS analysis of this sample reveals that the high activity is derived from the formation of active Ni-Co oxyhydroxide phase (NiIII-CoIIIOx(OH)) on the surface of the bimetallic Ni-Co HPi electrode. These results indicate the promising potential of nanotubes-assembled metal phosphate nanoarchitectures for electrocatalytic applications.

Biography:

Yusuf Valentino Kaneti is an Advance Queensland Industry Research Fellow at the Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland

(Australia). He received his PhD degree from the University of New South Wales. He has previously obtained Endeavour Australia Fellowship (2015) and JSPS Fellowship (2016) from Australian and Japanese governments, respectively. His research interest is on the fabrication of nanoporous materials for energy and sensing applications. He has published >100 peer-reviewed journal articles, including 14 Highly Cited Papers and 1 Hot Paper. He currently serves as an Editorial Board Member of Batteries, Crystals and Gases (MDPI).

Hygroscopic insulator field effect transistors for sensing

Soniya D. Yambem[1*]
Joshua N. Arthur[1]

[1]School of Chemistry and Physics and Centre for Materials Science, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia

Abstract

In the last decade, there has been significant progress in bionic devices such as electronic skin. For these devices to be fully integrated in the human body, bioelectronic interfacial devices that can act as transducers between the human body and electronic components are crucial. The challenge lies in the difference between the intrinsic modes of sending signals in electronic devices and the biological world. Most electronic devices send signals through flow of electrons, while biological systems exchange information through flux of ions such as Na+, K+, etc. and protons. There is considerable interest in developing bioinspired devices for bioelectronics.

We will present our work on hygroscopic insulator field effect transistors (HIFETs) for sensing and bioelectronics. HIFETs are an all-solid state, low voltage operating organic thin film transistor (OTFT) with promising applications in sensing. Sensing using HIFETs is done mainly through modification of the gate electrode, which could lead to lower conductivity of gate electrodes. Our investigation showed there is a threshold conductivity, above which conductivity does not play a significant role in performance of HIFETs. This indicates that the gate electrodes can be modified to incorporate sensing elements without compromising transistor performance. We explored different gate materials for HIFET sensors. We also developed stable gate electrodes of cross-linked PEDOT:PSS and studied HIFET characteristics and sensing. More recently, we developed a method to study sensing mechanism in HIEFTs using confocal fluorescence microscopy. This method is easily translatable and applicable to many OTFT sensors. Further, we will present ion sensing using HIFETs.

Biography:

Soniya is a device physicist with extensive experience in fabricating flexible electronic devices. At QUT, Soniya's work is focused on optoelectronic and bio-electronic interface devices for developing sensors and biosensors for bioelectronic and bionic applications. Before this, Soniya worked as a post-doctoral researcher at Centre for Organic Photonics and Electronics, University of Queensland. In 2015, Soniya was awarded QUT's Vice Chancellor's Research Fellowship and transitioned to a faculty position in 2018. Soniya completed her Ph.D. at the University of Houston (UH), USA. She also holds two Master degree in Physics; one from UH and another from University of Delhi, India.

Microcellular foams of polymer/cellulose nanofiber composites

Kim Dongho[1]
Jisuk Lee[1]
Yuta Hikima[1]
Long Wang[2]
Masahiro Ohshima[1*]

1) Dept. of Chemical Engineering, Kyoto University, Japan

2) Ningbo Institute of Materials Technology & Engineering (NIMTE), China

Abstract

Incorporating micro-/nano-particles is one of the most efficient approaches to reinforce polymers with desired properties. A typical reinforcement approach that has always been realized is to add inorganic particles. However, it would reduce the recyclability of the polymers. To increase the green nature of the polymers, we have been investigating a green strategy to add renewable and biodegradable cellulose nanofibers (CNFs) into several polymers, such as polypropylene (PP), polylactide (PLA), poly(butylene succinate-co-adipate) (PBSA), and poly(3- hydroxybutyrate-co-3-hydroxyhexanoate) (PHBH). These polymers could obtain well-dispersed hydrophobic-modified CNFs in polymer matrix by combining chemical surface modification and melt-compounding technology (so-called Kyoto process). These polymer/CNFs composites were shown to have a notable increase in the crystallization rate and melt elasticity at a low-frequency range, which drastically enhances the physical foaming behaviors of these polymer/CNF composites and provides the fine polymer foams with micro/nano cellular structures. These results demonstrated that CNFs were extraordinarily helpful in enhancing foamability, which is expected to be a green and sustainable filler for polymers.

Biography:

Ohshima started his academic career as an Instructor of Chemical Engineering at Kyoto University in 1986. Then, in 1994, he became an Associate Professor of Computer Science and Systems Engineering at Miyazaki University. Two years later, he returned to Kyoto University and became full Professor in 2001. Since then, he has been serving as a Professor of Chemical Engineering at Kyoto University and the Material Process Engineering laboratory leader. He received numerous awards in process control and polymer processing areas. He served as the dean of faculty of engineering Kyoto University for three years from 2018 to 2021.

(Photo)electrochemical Cells for Hydrogen and Hydrocarbon Production

Tsutomu Minegishi*

Research Center for Advanced Science and Technology, The University of Tokyo, Japan

Abstract

Photoelectrochemical (PEC) and electrochemical cells for water splitting and carbon dioxide reduction reaction (CO2RR) are the key technologies to achieve carbon neutral society.

In the PEC cell, photoelectrode absorb light and provide driving force for water splitting reaction. The most difficult issue for photoelectrode is to achieve both long absorption edge wavelength and large driving force. Cu(In,Ga)Se2 (CIGS) which is employed as an absorber in photovoltaic devices is one of the promising photocathode materials because of its long

absorption edge. However, its driving force for water splitting is not enough due to the small ionization potential. The solid solution between ZnSe and CIGS (ZnSe-CIGS) possess both long absorption edge of about 900 nm and large driving force of about 1.0 V. In the present study, we investigated introduction of tellurium during ZnSe-CIGS thin film deposition, and, consequently, increase grain size and lowering of optimal deposition temperature of ZnSe-CIGS film were found. Furthermore, the formation of composition gradient which is beneficial for charge separation thorough conduction band minimum gradient was observed. The ZnSe-CIGS photocathode prepared with tellurium introduction and composition gradient showed significantly increased incident photon-to-current conversion efficiencies.

The electrochemical cell with gas diffusion electrode (GDE) for CO2RR can produce useful chemicals efficiently. In the present study, Cu2O was examined as an electrocatalyst for CO2RR. A GDE composed of carbon paper coated with Cu2O showed C2H4 and C2H5OH production with Faradaic efficiencies of >50% and >20%, respectively, were observed under the optimized conditions for more than 20 hours.

Biography:

Project associate professor Tsutomu Minegishi received Ph.D from Tohoku University in 2008. He became a post-doctor in Prof. Kazunari Domen`s group of The University of Tokyo in 2008. He appointed as project assistant professor in 2009 and as associate Professor in 2015. His major research interests are development of semiconductor materials and devices for photocatalytic and photoelectrochemical direct synthesis of energy carrier including water splitting using solar energy.

Toughening of Glass by Imparting Ductility by Nanometals

Kenji Shinozaki[1,2*]
Liu Lei[1]

[1]National Institute of Advanced Industrial Science and Technology, Japan

[2]JST Presto, Japan

Abstract

Glass is an essential material in modern society, but its brittleness, which has long been a major issue, limits its structural applications. At its root cause, the brittleness of glass comes from the lack of a stable shearing mechanism and from the significant concentration of stress at the crack tip, which occurs due to highly elastic nature. Therefore, imparting the ductility to brittle oxide glass significantly improves its brittleness. Here, we focus morphology control of precipitated metal particles and clarify their roles in deformation and fracture. We have succeeded in significantly reducing the brittleness of metallic nanoparticles by dispersing them in glass with controlled size and dispersion morphology. For instance, ductile sub-micron-scale Ag particles were homogeneously dispersed in SiO2 glass using a simple method. The addition of a small amount of Ag particles (1.4 vol%) significantly changed the plastic deformation behavior of the glass by making it ductile. As a result, cone cracks were less likely to form, and radial cracks were prevented from propagating. Furthermore, crack bridging and deflection of ductile Ag particles, both of which increased the fracture surface energy, were observed following the dispersion of Ag particles. SiO2 glass is one of the most important oxide glasses, and increasing its ductility offers new material design approaches. The remarkable improvement in fracture toughness, i.e., 0.85 ± 0.2 MPam1/2 for the sintered

SiO2 glass and 2.01 ± 0.2 MPam1/2 for the 1.4 vol% Ag-precipitated SiO2 glass. This will contribute significantly to improving its applicability in numerous industrial applications.

Biography:

Kenji Shinozaki received a Ph.D. in Engineering at Nagaoka University of Technology in 2013. He was a Research Fellowships for Young Scientists of Japan Society for the Promotion of Science (JSPS) in 2013, and he worked as an Assistant Professor at Nagaoka University of Technology from 2013 to 2016. Since 2016, he has worked at National Institute of Advanced Science and Technology (AIST) as a researcher. His current research interest includes materials science and fabrication processing of glasses and glass-ceramics for mechanical and photonic applications.

Microwave Attenuation Effect of Carbon Nanofibers with Different Thickness

Hee-Jo Lee*

Department of Physics Education, College of Education, Daegu University, South Korea

Abstract

Carbon nanofibers (CNFs) as nanocomposites have widely attracted microwave absorbing materials due to low density, high strength, and excellent electrical properties. In addition, the materials' complex geometrical morphologies and good conductivity can enhance load resistance with integrated effects between the composite of CNFs and the electromagnetic (EM) wave, such as scattering, absorption, internal multi-reflection, and polarization. This talk presents the microwave transmission properties of carbon nanofiber (CNF) with three different micrometer-scale thicknesses. In the key experimental results, when the film of CNFs was thick, the signal transmission level (S21-magnitude) was significantly lower, and its phase (S21-phase) was shifted toward the low-frequency region. Furthermore, based on the experimental data, the electric permittivity of CNF was extracted and showed apparent differences depending on the thickness. In the analysis of EM fields, the microwave conductivity of CNFs linearly increased with the increasing thickness due to enhanced EM field coupling between the film of CNFs and the microwave transmission line (CPW line). As a result, this work demonstrated that the film of CNFs has a significant attenuation effect on signal transmission in the microwave regime (0.5-10 GHz), depending on micrometer-scale changes in film thickness.

Biography:

Hee-Jo Lee received Ph.D. in Electrical and Electronic Engineering from Yonsei University, Seoul, South Korea, in 2010. From March 2010 to August 2014, he worked in Electrical and Electronic Engineering, Mechanical Engineering, Yonsei University, as a post-doctoral researcher and a research professor. As a post-doctoral researcher, he also worked in Graphene Research Institute, Sejong University. Since September 2014, he is currently an associate professor in the Department of Physics Education, Daegu University. His main research interests are electromagnetic wave and field theory, computational electromagnetics, RF/microwave biomaterials and gas molecule sensing platforms, RF/microwave circuit modeling and characterization of carbon nanomaterials, including graphene, graphene oxide, and carbon nanofiber, and electromagnetic metamaterials.

Efficient functionalization of single-walled carbon nanotubes for dispersant-free colloidal dispersion and its electrical applications

Joong Tark Han[*1,2]

[1]Nano Hybrid Technology Research Center, Electrical Materials Research Division, Korea Electrotechnology Research Institute, South Korea

[2]Department of Electro-Functionality Materials, University of Science and Technology, South Korea

Abstract

Surface functionalization of carbon materials such as carbon nanotubes (CNTs) and graphene nanosheets facilitates their dispersion in solution, without using a dispersant, by overcoming the van der Waals interactions between the nanoscale carbon materials1-3. Unfortunately, permanent functionalization can compromise some of the electrical properties which make these carbon materials so valuable. In particular, single-walled CNTs (SWCNTs) tend to be shortened and damaged under harsh oxidation conditions because their curved surfaces have higher reactivity than the graphene basal plane. In this talk, we present the rational oxidation method of SWCNTs via acid treatment by minimizing defect formation on the surface. Importantly, the structure of the oxidized SWCNTs (Ox-SWCNTs) could be recovered by chemical, thermal, photothermal, or solvothermal reduction, enhancing the electrical conductivity of the Ox-SWCNT films from ~100 to ~1000 S cm−1. The electrical conductivity, Raman analysis, and XPS data all demonstrate the structural recovery of highly oxidized SWCNTs without compromising their electrical or electrochemical performances. Our results demonstrate that remarkable electrical or electrochemical performances were obtained after deposition of SWCNT inks or pastes that were dispersed in water and various organic solvents (without additional dispersant). Supercapacitors and LIB cathode electrodes using Ox-SWCNTs and reduced Ox-SWCNTs showed high electrochemical performances compared to those employing pristine SWCNTs. The high solution dispersibility and structural recovery of oxidized carbon materials are expected to facilitate their application as electrical or electrochemical components in next-generation devices.

Biography:

Joong Tark Han received his Ph.D. in Chemical Engineering from Pohang University of Science and Technology (POSTECH) in 2005. He is currently a principal researcher in the Nano-Hybrid Technology Research center at Korea Electrotechnology Research Institute (KERI). His research interests are in exploring nanostructures and electronic structures of electrical nano-materials such as nanocarbon materials (carbon nanotube, graphene, etc.), nano-metal, metal oxide nanoparticles, for future smart electric devices.

Colorless and Transparent Polyimides

Chang-Sik Ha

Department of Polymer Science and Engineering, School of Chemical Engineering, Pusan National University, Busan 46241, Korea

Abstract

Transparent polymers are being considered as the key materials for flexible displays in various application areas including transparent substrates. The essential requirements for an optically transparent polymer for plastic substrates are to have a high glass transition temperatures

(Tg) for thermal processing, excellent optical transparency in the UV-visible wavelength range, and film-forming process compatibility, etc. But, perhaps, optical transparency at very high processing temperature is arguably the primary requirement. Among those high Tg polymers, aromatic PIs have been used in a variety of advanced electric and microelectronic devices for their simple two-step manufacturing processes. Conventional aromatic PIs, however, have deep colors and poor optical transmittance due to the intra- and inter-molecular charge-transfer (CT) interactions between the electron donating diamine and electron-accepting aromatic dianhydride, which considerably restricted their application in microelectronic and optoelectronic engineering, where colorlessness is an important requirement are considered. Many research attempts have been made for improving PIs' optical transparency through rational structural modification without compromising their excellent thermal and mechanical properties. Successful synthetic methodologies include the incorporation of fluorine atoms and the employment of alicyclic dianhydrides or diamines, etc. These structural adjustments could loosen the interchain packing, disrupt the conjugation, inhibit the formation of CT complex, and thereby leading to the formation of colorless PIs(CPIs). In this presentation, a few examples on the novel CPIs developed in my laboratory will be discussed.

Biography:

Chang-Sik Ha received his B.S. in Chemical Engineering from Pusan National University (PNU), Korea (1978) and his M.S. and ph.D. degrees in Chemical Engineering from Korea Advanced Institute of Science and Technology(KAIST), Seoul, Korea (1982 and 1987, respectively). He was a professor at the Department of Polymer Science and Engineering, PNU from 1982 to 2021. He served as a Vice President of PNU, and the President of the Society of Adhesion and Interface, Korea. Now, he is a Distinguished Professor of PNU. His research interests are Polyimides and Polysilesquioxanes, Organic/Inorganic Nanohybrid Materials, and Mesoporous Organosilicas, and so on.

Two UV plasmonic devices by high-performance epitaxial Al metasurfaces - an ultrasensitive photodetector and a surface-enhanced resonance Raman spectroscopic (SERRS) biosensor

Abhishek Dubey[1]
Ragini Mishra[2]
Yu-Hung Hsieh[2,4]
Chang Wei Cheng[3]
Bao-Hsien Wu[1]
Lih-Juann Chen[1]
Shangjr Gwo[2,3,4]
Ta-Jen Yen[*1]

[1]Department of Material Sciences and Engineering, National Tsing Hua University, Hsinchu Taiwan.

[2]Institute of Nanoengineering and Microsystem, National Tsing Hua University, Hsinchu Taiwan.

[3]Department of Physics, National Tsing Hua University, Taiwan.

[4]Research Centre for Applied Science, Academia Sinica, Taipei, Taiwan

Abstract

Plasmonics-based devices have been intensively explored in visible and infrared regimes, but scarcely demonstrated in the wide UV regime, mainly because of constrained optical properties of materials. By using epitaxial Al metasurfaces, herein we report two unprecedented plasmonic

applications in UV regimes- an ultrasensitive photodetector and a surface-enhanced resonance Raman spectroscopic (SERRS) biosensor. For the first UV plasmonic device, we demonstrated ultrasensitive photodetector with a maximum detectivity (1.48 × 1015 cm Hz1/2 W-1) at the on-resonance wavelength of 355 nm. broad bandwidth photodetection through the entire UV regime, and a fast temporal response with a rise time of 51 ms and a fall time of 197 ms, respectively. For the second UV plasmonic device, we presented an SERRS biosensor. Such a UV SERRS biosensor not only exhibited high signal to noise ratios, but also recorded an SERRS enhancement factor up to 106 for extremely thin layer of adenine of 1nm thick. In addition to this egregiously high EF factor, we further exhibit that our SERRS substrate is capable of detecting the single base mutation in the 12-mer ss-DNA.

Biography:

Ta-Jen YEN received his doctoral degree from UCLA in 2005 and then joined the department of Materials Science and Engineering (MSE) of National Tsing Hua University (NTHU), Taiwan. Currently, he is also a vice president at NTHU and a fellow of SPIE. Prof. YEN's research interests include, 1. Metamaterials, 2. Plasmonics, 3. Nanomaterials, and other related fields.

Surface-functionalized vesicle carriers: Towards a modular targeting drug delivery system

Thorsten Heidelberg*
Goh Ean Wei
Rusnah Syahila Duali Hussen

Chemistry Department, Faculty of Science, University of Malaya, Malaysia

Abstract

Drug-resistances and imperfect medical selectivity demand for the development of new medical drugs. Close linkages of cellular processes across species borders, however, place high obstacles for new active compounds and frequently cause unwanted side effects for traditional medicine. In order to address selectivity constraints, a variety of delivery systems for drugs have been proposed, aiming for a direction of the active component to target cells. A promising delivery system can be found in vesicular surfactant assemblies. These practically reflect miniature cellular structures, which shield the active ingredient from unwanted interactions. Membrane fusion processes, on the other hand, enable the transfer of the active ingredient into a target cell. The direction of the drug carrier towards the cellular target can apply specific antigen-receptor interactions. Such an approach, however, requires an efficient and lasting biofunctionalization on the exterior vesicle surface.

Aiming for a targeting drug delivery system, we have functionalized biantennary glycolipids for a click-chemistry based coupling with complementary functionalized biological antigens. The chosen surfactant design aims for maximum stability of lamellar assemblies and strong intermolecular forces, preventing a leaching of biological recognition anchors from the assembly. Incorporation of a charge to the otherwise non-ionic surfactants helps to control the assembly size and stabilizes vesicles from unwanted Oswald ripening, thereby ensuring a homogeneous distribution of an encapsulated drug. The coupling of antigens after formulation of the drug carrier maximizes antigen-efficiency and enables a modular delivery system based on the use of different antigens.

Biography:

Thorsten Heidelberg studied chemistry at the University of Hamburg, Germany. After his Ph.D. in synthetic carbohydrate chemistry, he spent time as a postdoctoral researcher in New York and in France, before joining a startup company on hard-particle based nanotechnology. He joined the University of Malaya as lecturer in 2006. His current research is focusing on the synthesis of carbohydrate-based surfactants and their application for the creation of nanosized drug carriers.

Titanium-doped Binary Strontium-Copper Oxide as a High-Performance Electrochemical Pseudocapacitive Electrode Material

Hasi Rani Barai[1*]
Paritosh Barai[2]
Sang W. Joo[1]

[1]Department of Mechanical Engineering, Yeungnam University, Gyeongsan 38541, South Korea

[2]Department of Biochemistry and Molecular Biology, Primeasia University, Dhaka-1213, Bangladesh

Abstract

Ti-doped SrCu2O2 (TSCO) is prepared using solid-state chemical reaction to apply as electrochemical pseudocapacitors. Crystallographic, Spectroscopic, and Morphological study of prepared TSCO confirmed the crystallinity. Electrochemical test of the synthesized electrode material; TSCO demonstrate specific capacity (Cs) of ca. 1167.6 and 661.8 F/g at a scan rate of 5 mVs-1 and 0.02 A/g applied current density, respectively which is much higher than the un-dopped SCO. The increment of the specific capacity value can be explained by the insertion of Ti as dopped material in the SCO which is simultaneously intensify the rate of ion intercalation/de-intercalation during the charging/discharging (CD). Even the cycling stability of TSCO was found excellent with only 4.4% decrease after 10000 CD cycling. Therefore, TSCO can be used as an outstanding electrode material for the high performance super capacitance applications to make the energy storage.

Biography:

Hasi R. Barai, RLRC-YU is the professor in school of Mechanical and IT Engineering, Yeungnam University, Gyeongsan, Korea, from 2015. She also worked as a postdoctoral research fellow in Chemistry and nanoscience, Ewha Womans University, Seoul, Korea and in KCAP-Korea centre for artificial photosynthesis, Sogang University, Seoul, Korea. She received her Ph.D. in Physical Organic Chemistry in Inha University , Korea, MS (Physical chemistry) in Dhaka University, Bangladesh. She is the active and life-time member in ACS-American Chemical Society, USA, KCS-Korean Chemical Society, Korea, BCS-Bangladesh Chemical Society, Bangladesh, Geomate-Geotechnique, construction, materials & environment, Japan. Dr. Barai is the Guest Editor in Polymers (SCIE-4.329 MDPI journal) and also the editor in another two Engineering international renowned journals. Dr. Barai has a number of presentations, international scientific publications and reviewer in some renowned journals. Leadership research mentor in major fields nanotechnology and nanomaterials, materials preprocess, electrochemistry and nanomaterials, supercapacitors.

End of Day 05 Parallel Session I

Oral Presentations

Injectable thixotropic hydrogels for tissue regeneration

Boiziau C [1*]
Barthelemy P [2]
Boeuf H [1]
Sindhu KR [1]
Rathore A [1]
Bansode N [2]
Rey S [1]

[1] Inserm, Univ. Bordeaux, BioTis UMR 1026, Bordeaux, France.

[2] Inserm, Univ. Bordeaux, ARNA UMR 1212, Bordeaux, France.

Abstract

Low molecular weight hydrogels (LMWHs) formed by self-assembly of small molecules interacting by non-covalent interactions are of increasing interest because they are soft, easy to use and injectable. In the context of tissue engineering, these properties define them as suitable materials that can stimulate tissue repair. Different hydrogels have been studied, with particular emphasis on the thixotropy property, for in vivo applications such as sustained drug release, angiogenesis-promoting biomaterials, or local cell delivery. To this end, disulfide bonds were introduced in the hydrophobic segment of a new glycosylated nucleoside based bola-amphiphile (GNBA); thiol-disulfide exchange reactions were used to achieve sustained release of a thiol-containing protein. Other GNBAs have been shown to promote blood vessel development due to the local release of an angiogenic degradation product. Potential applications of such injectable hydrogels will be discussed.

Biography

Claudine Boiziau was born in 1964 in France. After graduation as Engineer of ENSTA-ParisTech (Paris, France) in 1988, she received the PhD degree of Molecular and Cellular Pharmacology from the University P&M Curie, Paris, France in 1991. She was recruited as a researcher at Inserm (a public research organization dedicated to human health) in 1993. Since then, she is working as a researcher at the University of Bordeaux, France. Since 2013, she has joined the Inserm unit BioTis, working on biomaterials for tissue regeneration. Her research focuses on host inflammatory responses after implantation of medical devices, and biomaterials designed for regeneration.

Humidity responsive self-actuated cellulose-based materials

Shiva Khoshtinat*
Valter Carvelli
Claudia Marano

Politecnico di Milano, Italy

Abstract

Toward the production of humidity-responsive self-actuators, the humidity actuation in some plants (e.g. pinecones) has been mimicked. For this purpose, a cellulose-based material (cellulose acetate), renowned for its hygroscopic behavior, was used as a lamina for bi-layered selfactuators. The hygroscopic properties of the membrane material were evaluated via gravimetric measurement and thermomechanical analysis, at constant temperature (T = 25 °C), in a wide range of relative humidity (RH = 21–76%). The "variable surface concentration" model [1] was used for the description of sigmoidal moisture diffusion resulted from the gravimetric measurements. The interpolation of this model to the experimental data allowed to have a polynomial function of relative humidity for the concentration at saturation (Csat), with constant values of: the diffusion coefficient D = 3.35×10-6 mm2 ⁄s, and the relaxation factor β = 0.026 s -1 [2] . Thermomechanical Analysis provided the measurement of the induced hygroscopic expansion (εhygro) resulting in a polynomial function of relative humidity. The coefficient of hygroscopic expansion (α) has then been obtained by the ratio of εhygro and Csat as function of relative humidity. These properties were used to build a COMSOL Multiphysics® finite element model to predict the sigmoidal moisture diffusion, moisture concentration, induced hygroscopic expansion, and the relevant induced bending deformation ofself-actuated bi-layersfor different levels of relative humidity. The results of the finite element model reproduce the real-time hygro-mechanical response of bi-layered composite consisting of a cellulose acetate membrane coupled to a nonhygroscopic substrate.

Biography:

Shiva Khoshtinat is a third-year material engineering Ph.D. student at Politecnico di Milano. She received a bachelor's degree in civil engineering from Babol Noshirvani University of Technology (Iran) and a master's degree in architectural design from Università degli Studi di Firenze (Italy). Currently,she is involved in an interdisciplinary Ph.D. project aiming to study humidity responsive materials. She is interested in biomimicry of structure, material, and behavior of natural organism for sustainable design.

Pulsereverseplatingandtheprocessofbuildingabathtoproducenanocompositecoatings

Statharas D
Weston D*

Department of Engineering, The University of Leicester, Leicester, UK

Abstract

Pulse reverse plating (PRP) has been an important step towards electroplating advanced materials. PRP has demonstrated that it is possible to plate both alloys and composites directly on a substrate. However, the balance of chemistry, electro-chemistry, fluid dynamics and processing is very delicate. Absolute control of the process has yet to be achieved but a

process from which plating baths can be built has emerged. The process presented can be used to build electrodeposition baths for depositing both alloys and composites on a substrate. The process provides with the capability of troubleshooting a bath while it is being built. This allows for the control of smaller groups of parameters at the time. Fixing issues while the bath is being built enhances both the scientific knowledge, due to the improved understanding of the process, and the end goal of the process which is always the deposition of a functional and robust coating. Additionally, this process allows for the exploration of bath 'tolerances' which can facilitate industrial adaptation and use of improved coatings. Potentially, through this process, coating systems can emerge that will either improve existing systems or replace working systems that have negative impact on both the health of the people involved and the environment (i.e. hard chrome).

X-ray absorption and emission spectroscopies to address functional mechanisms in batteries materials

L. Simonelli

Alba Synchrotron, Carrer de la llum 2-26, 08290 Cerdanyola del Vallès, Catalonia, Spain

Abstract

Increasing the contribution of renewable energy sources is necessary to meet the fast increase of global energy needs and match the CO2 reduction targets. In order to address these challenges, intensive research efforts are ongoing both in energy harvesting and storage technologies such as solar panels, fuel cells, supercapacitors and batteries. The latter are required to match the energy demand and supply; in fact, batteries are by far the most ubiquitous energy storage technology currently employed.

Synchrotron x-ray spectroscopies have played a key role in the continuous development and breakthroughs in battery science, thanks to their capability to provide accurate information on electronic structure of the redox active element, local structure, and morphological information under operando or cycling relevant conditions. X-ray absorption and emission spectroscopies are highlighted for addressing battery materials, where the intrinsic complex nature of such materials often strictly requires a multi-techniques approach. The relevance of exploiting a wide energy range and multi-techniques approach, as well as the potential interest on imaging is presented [1-3].

Plasticity, Fatigue and Microstructural Effects in Polycrystalline Metallic Alloys

Jean-Charles Stinville[1*]

[1]Materials Science & Engineering, University of Illinois at Urbana-Champaign, IL, USA

Abstract

With increasing applied stress, metallic materials experience irreversible deformation, manifested in localized plasticity that results in unexpected fatigue failure upon repeated cycling. Recent advances in accelerated fatigue testing, in-situ electron microscopy, digital image correlation methods, and multi-modal data analysis have been integrated to quantitatively characterize the evolution of these plastic localization events at the nanometer scale over large fields of view in relation to material crystal structure and microstructure.

Statistical analyses of plastic localization events for a large collection of metallic materials with face-centered cubic, hexagonal close-packed, and body-centered cubic structures have been performed. Relations between macroscopic mechanical properties and the plastic localization events are uncovered. For instance, It is observed for the first time that the amplitude of slip localization during the first cycle of loading can predict the fatigue strength of fcc, hcp, and bcc metallic alloys. This relation is utilized to guide the design of new alloys.

Biography:

Jean-Charles Stinville is an assistant professor in the prestigious Materials Science and Engineering Department at the University of Illinois at Urbana-Champaign. His research focuses, amongst others, on the characterization of deformation processes for mechanical properties prediction and design of novel metallic materials. He plays an important role in the Materials Science and Engineering Department's future directions in metals and materials characterization for extreme environments. He is a recipient of the 2016 Hetényi Award, which is given annually for the best research paper published in Experimental Mechanics.

Interrogating the electronic structure of diketopyrrolopyrroles using femtosecond laser spectroscopy

TAA Oliver*

School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

Abstract

Diketopyrrolopyrroles (DPPs) are a popular class of electron-withdrawing unit in optoelectronics. When combined with electron donating side groups such as thiophenes, they form a large class of donor-acceptor molecules. There has been a recent surge in studies investigating the structure-function relationship of DPP molecules and polymers to inform their use in a range of applications, but very few of these address the underlying electronic structure responsible for the observed properties. Using transient absorption spectroscopy with 22 fs pulses and ab initio calculations, the electronic structure of three thiophene-based DPPs was investigated: a monomer, dimer and a polymer. The two low-lying electronic states of the DPP molecules studied can be described as optically bright or dipole forbidden (dark) in character. Despite this, in our transient absorption data, we observed vibrational wave packet signatures arising from both the bright and dark excited states. The dark state wave packets arise from nuclear motions induced at a linking conical intersection with the bright state. Despite the similar electronic structure, and conserved character of the electronic states, different photophysical dynamics were observed for the three systems which is entirely due to the energetic re-ordering of electronic states upon elongation of the aromatic p-network.

Biography:

Tom Oliver is a Royal Society University Research Fellow at Bristol with a proleptic Associate Professor appointment. He received his PhD from the University of Bristol in 2011 under the supervision of Prof. Mike Ashfold FRS. He was then a postdoctoral research fellow at UC Berkeley with Prof. Graham Fleming FRS, where he pioneered the two-dimensional electronic−vibrational spectroscopy technique. His research interests currently include ultrafast dynamics of materials, non-radiative relaxation dynamics in protein and solution, development of novel 2D optical spectroscopies, photoprotection, and repair in DNA and higher plants.

Small-Nanostructure-Size-Limited Phonon Transport within Composite Films Made of Single-Wall Carbon Nanotubes and Reduced Graphene Oxides

Qing Hao1*
Qiyu Chen1
Xiaolu Yan2
Leyuan Wu2
Yue Xiao1
Sien Wang1
Guoan Cheng2
Ruiting Zheng2

[1]Department of Aerospace and Mechanical Engineering, University of Arizona, Tucson, AZ 85721, USA

[2]School of Nuclear Science and Technology, Beijing Normal University, Beijing 100875, P. R. China

Abstract

In this work, flexible and lightweight nanocarbon composite films consisting of reduced graphene oxides (rGOs) and single-wall carbon nanotubes (SWCNTs) are synthesized and studied for their in-plane thermal conductivities. With the adding of SWCNT-graphene junctions in the composite films, the inplane thermal conductivities of these composite films are found to follow the trend of the specific heat of graphene from 100 K to 400 K, i.e., monotonously increasing at elevated temperatures. Such a trend can often be found within amorphous solids but has seldom been observed for nanocarbon. This unique temperature dependence of thermal conductivities is attributed to the largely restricted phonon mean free paths (MFP) within the graphene sheets that mainly contribute to the in-plane thermal transport. This is aligned with the so-called small-nanostructure-size (SNS) limit, at which the phonon MFP Λ is fully confined by the nanostructure size. The highest in-plane thermal conductivity among samples with different synthesis conditions is 62.8 W/m·K at 300 K. Such a high thermal conductivity, combined with its unique temperature dependency, can be ideal for applications such as flexible film-like thermal diodes based on the junction between two materials with a large contrast for their temperature dependence of the thermal conductivity.

Biography:

Qing Hao is an Associate Professor in Aerospace and Mechanical Engineering at the University of Arizona. He joined the University of Arizona (UA) in 2011. His current research efforts electrothermal studies of power electronics, thermoelectrics, boiling and condensation, measurements and engineering applications of graphene and other two-dimensional materials. He received the AFOSR YIP Award and NSF CAREER Award. At UA, he received the Craig M. Berge Dean's Fellow in 2020. He was among the 70 Invitational Fellows for Research in Japan for Year 2021.

Exploring Optical Properties in Perovskites-Based Solar Cells: Theoretical Insights from Hybrid DFT, GW and BSE

Saswata Bhattacharya

Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016

Abstract

Materials for optoelectronic applications have received a lot of attention worldwide in a variety

of fields over the past several decades. Recently, perovskites have also been revolutionized the field of emerging photovoltaic and optoelectronic technologies. Understanding these materials at the theoretical perspective is never been easy because of the exchange-correlation functional that needs to be carefully analyzed in the light of electron's self-interaction error and spin-orbit coupling (SOC). Conventional first principles based simulation under the framework of Density Functional Theory (DFT) with local / semilocal functionals (viz. LDA or GGA), is not sufficient to determine the excited state properties. Therefore, to study the excited state properties, we employ a general framework of the firstprinciples calculation under many-body perturbation theory (MBPT) approach. These approaches of beyond DFT formalism are essential for a quantitative description of photoemission, inverse photoemission and light absorption experiments in these materials. In this talk, I will give a broad overview with various examples[1-10], where the conventional DFT calculations fails and how many body perturbation theory viz. one particle Green's function (GW) method and higher order Green's function techniques (Bethe-Salpeter Equation) help in addressing the excited state properties especially in the context of capturing excitonic properties of the materials. This state-of-the-art methods have permitted us to simulate optical absorption spectra and various properties (viz. refractive index, extinction coefficient, reflectivity, absorption coefficient, loss spectrum etc.) with unprecedented accuracy with respect to the experiments.

PHYSICAL PROPERTIES OF REFRACTORY CARBIDES UP TO 5000 K

Alexander Savvatimskiy*
Sergey Onufriev

Joint Institute for High Temperatures Russian Academy of Sciences, Moscow, Russia

Abstract

A high-speed method for measuring the thermophysical properties of the most refractory substances (carbides) in the liquid phase at high temperatures has been developed and implemented. Since the duration of heating by a current pulse is millionths of a second, significant financial costs are not required to provide expensive equipment for long-term high temperature maintenance. In addition, refractory crucibles are not needed to preserve the liquid phase for further investigation of properties. Due to the short duration of heating, the sample in the liquid state does not change its shape and retains its position in space for a dozen microseconds. This allows for this time, using high-speed oscillography, to obtain the properties of refractory substances in the liquid state.

Experimental results of the physical properties for refractory carbides (ZrC; ZrC+C; TaC; HfC; TaC+HfC) at high temperatures are presented. The samples were thin plates with a thickness of about 150 microns, which were heated by a current pulse of about 20-30 kA during 5-10 microseconds. The properties were measured: the input Joule heating energy (enthalpy H), specific heat Cp, electrical resistance R. Measurement error H; Cp; R – 7%; 15%; 5%, accordingly. The temperature range studied included the melting region (from 3850 to 4300 K for these carbides) and the liquid phase, up to 5500 K.

The temperature was measured by an optical method with a pyrometer based on a high-speed photodetector PDA-10A (Thorlabs) using a known emissivity. To study ZrC+C, samples were used in the form of a wedge-shaped model of a black body (developed in the USA by Mendenhall back in 1911), therefore, knowledge of the emissivity was not required. In this

experiment, ZrC+C carbide covered two glass plates folded by a corner with a thin layer during magnetron sputtering.

The results obtained are necessary for the creation of thermal protection in the nuclear power industry and in the aerospace field.

Biography:

BORN: April 15, 1940, Moscow, Russia

NATIONALITY: Russian

EDUCATION: 1957 - Finished secondary school in Moscow, 1957-1959 - Laboratory assistance in All-Union heat-engineering Institute, 1959-1966 - Undergraduate, Moscow Power Engineering Institute, speciality: Thermophysics, 1975 - Ph.D. in experimental thermophysics. Thesis: "Measurements of melting heat and resistance of liquid refractory metals at melting region under fast electrical heating". Institution of degree: Institute for High Temperatures RAS, 1999 - Highest Degree earned: Doctor of Technical Sciences in Thermophysics and molecular Physics. Thesis: "Experimental investigations of physical properties (metals, alloys and graphite) under microsecond electrical pulse heating", Institution of degree: Institute for High Temperatures RAS.

Controlled thermal expansion materials

Andrea Sanson[1*]
Alessandro Venier[1]
Qilong Gao[2]
Lei Hu[3]
Yongqiang Qiao[4]
Naike Shi[4]
Jun Chen[4]

[1]Department of Physics and Astronomy, University of Padua, Italy

[2]School of Physical and Microelectronics, Zhengzhou University, China

[3]School of Materials Science and Engineering, Nanyang Technological University China.

[4]Department of Physical Chemistry, University of Science and Technology Beijing, China.

Abstract

Thermal expansion, the tendency of materials to change in shape and volume in response to a change in temperature, is a significant problem for the many materials and engineering applications where thermal stability is required. Accordingly, the control of thermal expansion represents a challenge for materials design. In the last two decades, after the discovery of materials which display large negative thermal expansion (NTE) over a wide temperature range, the goal of controlling thermal expansion has become feasible and the number of studies on this topic has grown rapidly. In this contribution, the most promising methods to tune the thermal expansion are introduced, including chemical intercalation, chemical substitution, nano-size or magneto-volume effects. The physical-chemical phenomena associated with the thermal expansion changes are described and our recent advancements presented [1-5].

Biography:

Andrea Sanson is Associate Professor of Experimental Condensed Matter Physics and the Department of Physics and Astronomy of the University of Padua, Italy, and Academic Board

Member of the PhD Course in Science and Engineering of Materials and Nanostructures. His research activity is focused on the structural and dynamical aspects of condensed matter physics, specifically with regard to controlled thermal expansion materials, ionic conductors, ferroelectrics, semiconductors, and more in general, crystalline materials of functional interest. Author/co-author of about 90 publications in indexed scientific journals (12 as single author + 21 as first author, h-index=25 and ~2000 citations), he is Editorial Board Member of the journals Materials (MDPI) and Microstructures (OAE Publishing).

The microscopic nature of the anomalous thermal expansion phenomenon

Andrzej Łapiński

Institute of Molecular Physics Polish Academy of Sciences, Poland

Abstract

Many materials expand in three directions when heated. Such a phenomenon is called positive thermal expansion, and it is due to the increased anharmonic vibration of bonds. However, some materials show the opposite trend in thermal behavior. This anomalous thermal expansion phenomenon is known as negative thermal expansion (NTE).

NTE materials have attracted significant interest due to their potential applications as thermomechanical sensors, high-performance explosive materials, fiber optic systems, packaging materials for refractive index gratings, actuators, high-precision optical mirrors, and sensors. When designing materials with desired thermal properties, a proper understanding of the causes and mechanisms of thermal expansion is essential.

Many factors may cause the NTE effect: magnetic and ferroelectric phase transitions, rigid unit modes, geometrical variations, electronic effects, magnetostriction, steric hindrance effects [1-3]. In discussing the microscopic nature of the phenomenon of anomalous thermal expansion, particular attention will be paid to the role of transverse vibrations and structural distortions [4]. The anomalous thermal expansion can be explained by the following mechanisms: accordion motion, the sliding of layers, jack motion, fencing mechanisms, scissor effect, pedal-wheel motion [4-6].

Studies of the crystallographic structure and infrared and Raman spectroscopy are used to discover the microscopic nature of this unique phenomenon. During the presentation, the results obtained after the analysis: of the expansivity indicatrix along principal axes, the percentage of voids in the crystal, the computed electrostatic potentials, the Hirshfeld surface and fingerprint plots, the total lattice energy partitioned into its electrostatic, polarization, dispersion, and repulsive contributions will be presented and discussed.

Biography:

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FEM modeling of the deformation behavior of Ti–6Al–4V lattice structures based on cross-sectional imaging

Michał Doroszko[1*]
Anna Falkowska[1]
Andrzej Seweryn[2]

[1]Bialystok University of Technology, Poland
[2]Gdańsk University of Technology, Poland

Abstract

The paper presents the finite element modeling of the deformation behavior of cellular structures obtained by the additive manufacturing. The investigation uses biomedical Ti-6Al-4V titanium alloy with various relative densities. To simulate the process of tensile strain of the materials, realistic geometric models were used. In order to reconstruct the geometry of the mesostructures, computed tomography and microtomography were used, which allowed to obtain two accuracy levels of the mapping details of the investigated structures shape. Taking into account the true stress-strain of the material in the computational model makes it possible to simulate the deformation process of cellular structures until the fracture initiation. Based on the performed calculations using the finite element method, the stress and strain fields in lattice structures were received and analyzed. The relationship between the mesostructures shape and their macroscopic mechanical properties was studied. The influence of the accuracy of the lattice structures shape mapping on their mechanical properties and stress and strain fields was also analyzed. Based on the research, fracture initiation zones in diamond lattice structures were indicated. In the end, the results of the finite element modeling were verified by experimental results.

Biography:

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Laser-textured Ti6Al4V alloy: tribological response under dry conditions and lubricated with Hank's solution

Marjetka Conradi

Institute of metals and technology, Lepi pot 11, 1000 Ljubljana, Slovenia

Abstract

Nanosecond Nd-YAG laser with 1064 nm wavelength was used to define different morphologies of Ti6Al4V surface: lines, crosshatch with varying scan-line separation (Δx = 100, 180, 280 μm) and dimples. The influence of the surface morphology, texture density and orientation (parallel, perpendicular and at 45o) on the friction/wear under dry and lubricated (Hank's solution) sliding conditions was analyzed to evaluate the specific laser texturing of Ti alloys for biomedical applications. Under dry conditions, significantly lower steady-state coefficient of friction (COF) for dimple textured surface was observed in comparison to lines and crosshatch pattern as well as to as-received Ti6Al4V surface. In Hank's solution improvement in terms of

steady-state COF was observed after removal of the bulges around laser-textures for line and crosshatch patterns, especially when using smaller texturing density. However, for dimple textured surface high concentration of generated wear particles prevent dimples to act as oil reservoirs which resulted in higher friction than observed for non-textured surface or dry sliding. In terms of wear, combination of abrasive and adhesive wear mechanism was observed for all samples under both, dry and lubricated sliding conditions, with low density line and dimple patterns giving improved wear resistance. Thus, the most promising laser-texturing pattern for biomedical applications with a high risk for appearance of starved/dry-lubrication condition are low density line pattern oriented parallel or at 45° to the sliding direction and particularly dimple textured surface, where balance between wear particles generation, retaining within the contact and hiding in the cavities, is obtained.

Biography:

Marjetka Conradi obtained her PhD degree in physics in 2003 and is currently employed as a senior researcher at Institute of Metals and Technology and as assistant professor at University of Maribor. Main research topics: (i) Polymer (nano)composites (physical, mechanical properties/testing), (ii) Corrosion of metallic materials, (iii) Corrosion protection coatings, (iv) Biocompatible materials, coatings and (v) Surface (nano)structuring, tailoring surface properties for specific end-use.

BUILDINGS AND CONSTRUCTIONS FROM BUILDING WASTE MATERIALS IN ACCORDANCE WITH THE NEW CIRCULAR ECONOMY TREND

Monika Gwóźdź - Lasoń*

University of Bielsko-Biala, Faculty of Materials, Civil and Environmental Engineering, Institute of Civil Engineering, Poland

Abstract

The circular economy in the construction sector is key to increasing the reuse of waste materials. According to the plan of the European Commission, the construction sector is considered a priority for Circular Economy CE. Recycling of steel or concrete, blocks or bricks from completed construction and demolition investments makes it possible to reuse a very large amount of waste, and thus significantly reduce the adverse reactions of the construction industry to our planet. According to the currently promoted EEA trends, an appropriate circular CE approach is key to improving the quality of the environment. The issue analyzed in the article describes the possibility of using batch and non-batch scrap recycling for security systems, modernization, renovation or construction of engineering structures. The article discusses the possibility of using concrete with construction recycled aggregate to create elements strengthening the structure of the object for the calculated adverse effects that the structures undergo during the influences of the basin in the area of mining exploitation. The strength and physical parameters of new building materials from circular recovery, comparable to typical building materials, together with the analysis of their replacement and market value, may be the basis for a new trend in the design, execution and utility sectors of construction.

NEW ANTIMICROBIAL MATERIALS – HOPE FOR THE FUTURE

Iva Rezić*
Mislav Majdak
Maja Somogyi Škoc

University of Zagreb, Faculty of Textile Technology

Abstract

Today we face challenges in preservation of human health. Not only the viruses, but also the microorganisms present a big global threat to the world population. Therefore, the World Health Organization has emphasized that efforts in trying to find new solutions against drug resistant microorganisms are needed. Those include investigation and production of new materials with special functional coatings active against resistant microorganisms. Material engineers and textile scientists can much to offer – by applying metal nanoparticles the potentially active materials are obtained. Moreover, by using microcapsulae slow release of active substances into the environment can be acchieved. Such materials can be used in medical purposes, for protection and prevention of microbial growth. Our results have shown that efficient prevention against MRSA and MSSA strains can be achieved by careful optimization of nanoparticle mixture in the active coating. By this, new materials bring hope that the fight against dangerous microorganisms will be successfully finished in a near future.

Biography:

Iva Rezić PhD PhD was until the October 2020 a Vice-dean for scientific research at the University of Zagreb, Department of Applied Chemistry, Faculty of Textile Technology, where she leads a group of scientists in the field of chemical analysis and material sciences, and teaches in courses: "Analytical Chemistry", "Instrumental Analysis Methods", "Physical Chemistry", "Textile Chemistry" and "Computer Method Design of Experiment". She is a double doctor of science - in the field of natural sciences (analytical chemistry) and technical sciences (textile engineering). Professional competences she applies in management of projects and teams, with current focus on development of antimicrobial coatings and antimicrobial biodegradable products. She published 56 scientific papers, university textbooks and 5 chapters in scientific books.

ROLLING WITH ROUGH ROLLS: A POSSIBLE TECHNIQUE TO OBTAIN SUPERFICIAL NANOGRAINS

Carlos Camurri [1*]
Yasmin Maril [1]
Alejo Gallegos [1]

Department of Materials Engineering, University of Concepcion, CHILE

Abstract

316L stainless steel plates of 5 mm initial thickness, normalized at 900°C, were cold rolled with different reductions and number of passes by using roughs rolls with three different surface roughnesses. Subsequently, the rolled samples were annealed at low temperatures, in the range 200-400°C for 1 h in an effort to achieve superficial nanograins. The superficial grains formed on the surface (sized ~200-400 nm) were smaller than those below the surface; this behavior was caused by the rolling conditions that generate a continuous field of highly

superficial deformations, which act as many nucleation centers for nanograins during the subsequent annealing. The superficial recrystallization of the sample leads to higher superficial hardness and less wear than standard samples, ie, rolled with smoth rolls.

Biography:

Carlos Camurri , Metallurgical Engineer, MSc and DSc in Metallurgy is a Full Professor and Director of the Materials Department at the University of Concepcion, Chile. His interest area are Metal Forming, Mechanical Behavior of Materials and Process Simulation. He has over 70 papers in ex ISI reviews.

His main researches involves:

- Improve of the mechanical properties and corrosion resistance of lead base anodes for copper electrowinning.

-Effect of the impurities on cathodic copper on their ductility and wire drawing.

-Improve of the tenacity of steel grinding balls.

-Cold rolling with roughs rolls to obtain superficial nanograins.

Machine learning for classifying dislocation grain boundary interactions

Reeju Pokharel1*
Sumit Suresh 1
Saryu Fensin1
Nithin Mathew2
Ed Kober2

[1]Los Alamos National Laboratory, MST-8, United States

[2]Los Alamos National Laboratory, T-1, United States

Abstract

Understanding the interaction between dislocations and grain boundaries (GB) provides important insight into deformation mechanisms in polycrystals. When dislocations encounter a GB, it can act opaque, translucent, or transparent relative to the incoming dislocation. Depending on the type of interaction, dislocation pile-up or propagation may occur which in turn affects the accumulation of stress and strain fields at the local level. One of the main challenges in studying dislocation-GB interaction, both experimentally and computationally, lies in the difficulty in probing the vast parameter space occupied by different GB structures and their response when they encounter a dislocation. In this work, we have explored the applicability of data-driven models by generating training sets from molecular dynamics simulations of variety of GB structures and their interactions with dislocations. Highly sophisticated strain functional descriptors, which are geometric descriptors to identify unique atomic environments and describe their similarities, are used to characterize the local grain boundary structures. Using these microstructural descriptors as input features and dislocationGB reactions as output classes, we have demonstrated that machine learning based surrogate models can learn this complex and highly non-linear relationships to accurately classify dislocation-GB interactions in a computationally efficient manner. Once validated, the surrogate approximates will be incorporated into larger length scale models to enable highfidelity scale bridging for multiscale models.

Biography:

Reeju Pokharel is a staff scientist in the Materials Science and Technology Division at Los Alamos National Laboratory. She received her PhD in Materials Science from Carnegie Mellon University in 2013. Her research areas include non-destructive in-situ microstructure characterization (2D and 3D) of polycrystalline materials using high-energy X-ray and neutron diffraction, and 3D imaging using micro-computed tomography. She is also interested in utilizing experimentally measured microstructure evolution data to inform crystal plasticity simulations for damage modeling and is also utilizing machine learning methods for developing data analysis algorithms for real-time feedback during beamline experiments.

Topographical cues support enhanced secretory profiles in stem cells

Maribella Domenech*
Heizel M. Rosado

Department of Chemical Engineering and Bioengineering Program, University of Puerto Rico, USA;

Abstract

Surface topographical cues are a low-cost strategy to stimulate metabolic and protein expression changes in cells. Physical cues such as substrate stiffness and porosity are among the most studied properties shown to enhanced cell differentiation and invasive phenotypes. Yet other physical cues, such as surface wettability, roughness and patterns have been less studied but represent an untapped potential for mechanical stimulation of cells. In this study, an array of topographical cues on polystyrene (PS) films was used to evaluate its effect on the growth, morphology and secretome of tumor and mesenchymal stem cells. Topographies examined include surface roughness, depth, grooves and wettability. Cells were cultured on these arrays in culture media supplemented with low serum followed by cell quantification and morphology assessment using image-based analysis, and protein and exosome profiling using conditioned media. Results show that cells cultured in grooved micropatterns, and high-degree wettability surfaces resulted to have higher elongation and this in turn, correlated with enhanced metabolic activity of the cells of up to 5-folds compared to standard culture surface. This behavior was also associated with higher secretion of factors and exosomes (3 to 9 folds) as compared to flat surfaces. Differential expression analysis of secreted factors indicates that factors associated to immune modulation were the second most prominent in grooved micropatterns. For tumor cells, factors associated to cell growth and invasion were highly enhanced. Overall, groove micropatterns and high surface wettability are physical cues supportive of enhanced secretory capacity in cells.

Biography:

Maribella Domenech is a Professor in the Department of Chemical Engineering at University of Puerto Rico-Mayaguez (UPR-Mayaguez). She completed a bachelor majored in Industrial Biotechnology at UPR-Mayaguez, a M.S. and Ph.D. in Biomedical Engineering at University of Wisconsin-Madison. She has been a researcher and educator in the areas of chemical engineering and biomedical engineering with emphasis on the design of cell culture technologies for stem cell and cancer biology. She collaborates in leadership positions the multidisciplinary research centers: NSF- ERC-Cell Manufacturing technologies (CMaT) and the NSF-EPSCOR-Center for the Advancement of Wearable Technologies (CAWT). Ongoing research projects are focused on the development of culture and sensing technologies for personalized medicine applications.

In Situ Tensile Behavior of Hi-Nicalon Silicon Carbide Fibers Exposed to High Temperature Argon Plasma

Zhuang Liu[1*]
Jason M. Meyers[1]
Jeffrey Schindler[1]
Frederic Sansoz[1]
Ting Tan[2]
Douglas G. Fletcher[1]

[1]Department of Mechanical Engineering, University of Vermont, Burlington, VT 05405, USA

[2]Department of Civil and Environmental Engineering, University of Vermont, Burlington, VT 05405, USA

Abstract

Direct mechanical characterization of silicon carbide fibers in extreme hypersonic aerothermal environment is critical to the development of next-generation inflatable thermal protection systems that could enable delivery of large payloads to planetary surfaces. In this article, we report direct measurements of tensile properties in Hi-Nicalon silicon carbide fibers exposed to high temperature argon plasma exceeding 1100 oC using an in situ mechanical testing system integrated into a 30-kW inductively coupled plasma torch chamber simulating the hypersonic atmospheric entry conditions. As a comparison, ex situ tensile tests were performed on virgin Hi-Nicalon silicon carbide fibers in both ambient air and vacuum conditions. In situ thermal and optical imaging was used to obtain a real-time resolution of the thermo-mechanical events occurring on the fibers during the high temperature argon plasma exposure. It is found that the high-temperature tensile strength of Hi-Nicalon fiber tows exposed to argon plasma is 0.74 ± 0.19 GPa, which denotes a 59% reduction from the virgin fiber strength in ambient air (1.81 ± 0.19 GPa). Fractographic characterization by scanning electron microscopy shows that the substantial degradation of tensile strength in Hi-Nicalon fibers results from a reduction of fiber cross-section due to active surface attack from high temperature argon plasma.

Biography:

Zhuang Liu received his PhD degree in Mechanical Engineering in University of Vermont in 2021. He is a motivated researcher who dedicated his research in the field of study workability of advanced materials such as SIC fibers via novel experimental approaches. Dr. Zhuang Liu would like to promote his latest study upon in situ tensile test of Hi-Nicalon fibers under argon plasma.

Atomic-Scale Phonon Spectroscopy Reveals Emergent Interface Vibrational Structure of Superlattices

Eric R. Hoglund[1*]
De-Liang Bao[2]
Andrew O'Hara[2]
Sara Makarem[1]
Zachary T. Piontkowski[3]
Joseph R. Matson[2]
Joshua D. Caldwell[2]
Thomas E. Beechem[4]
John A. Tomko[1]
Jordan A. Hachtel[5]
Sokrates T. Pantelides[2]
Patrick E. Hopkins[1]
James M. Howe[1]

[1]University of Virginia, United States of America
[2]Vanderbilt University, United States of America
[3]Sandia National Laboratories, United States of America
[4]Purdue University, United States of America
[5]Oak Ridge National Laboratory, United States of America

Abstract

Perovskite oxides offer an abundance of properties with technological importance that are tunable by creating superlattices. Most research so far focuses on electronic properties, but such superlattices can also feature unique thermal properties, which are dictated by lattice vibrations. Here we combine atomic-resolution integrated differential phase contrast scanning transmission electron microscopy, vibrational electron energy-loss spectroscopy, and density-functional-theory calculations to probe the phonon spectra and oxygen atom positions for a series of SrTiO3-CaTiO3 superlattices with one to twenty-seven unit-cells per layer. We show that large-period superlattices feature bulk plus localized interface vibrational modes. As layer thickness decreases, the bulk modes disappear while the interface modes underpin the new material's phonon structure, which is also reflected in the macroscopic vibrational response measured by UV-Raman and Fourier transform infrared spectroscopy. This behavior correlates to period thickness reaching the length scale of TiO6 octahedral coupling at the interfaces, thus reflecting the dominant role of interfaces as materials sizes decrease and the need for spatially quantified structural and vibrational data to enable complete understanding of superlattice behavior.

Biography:

Eric graduated with his Ph.D. in Materials Science from the University of Virginia in 2020 following a B.S. in Materials Science from the NC State University. In his Ph.D. he used state-of-the-art scanning transmission electron microscopy and electron energy-loss spectroscopy to understand the relation between the structural, vibrational, and electronic state of interfaces in materials. Eric is currently a Postdoctoral Research Associate in the ExSiTE group at the University of Virginia continuing his study of interfaces and working to advance the use of scanning transmission electron microscopy as a tool for local thermal measurements.

The synthesis, characterization, and photophysical properties of terbium(III)-centered complexes with potential application as chemical sensors.

Justin Stace*
Avery Daniels
Ryan Gagnon
Yanike Mashimabi
Jacob Utley

Abstract

Three terbium(III)-centered species with potential application as chemical sensors were synthesized via a one-pot synthesis and isolated as analytically pure powders: Tb(phen)2(NO3)3 (phen = 1,10-phenathroline), Tb(22'bpy)2(NO3)3 (22'bpy = 2,2'-bipyridine), and Tb(pydm)3(NO3)3 (pydm = 2,6-pyridinedimethanol). Their identity is confirmed by FT-IR, elemental analysis, complexometric titration, and NMR spectroscopy. When the anhydrous solid or in water-free solution, these compounds exhibit the characteristic strong yellow-green luminescence of terbium(III) species, when excited by short wavelength ultraviolet radiation, in accord with the antenna effect. When exposed to water, or strong acid (HCl(aq)) the luminescence is quenched. The luminescence is restored by simply drying the sample at 110°C. The Tb(phen)2(NO3)3 is insoluble in all common solvents, although it forms optically-clear colloidal suspensions. However, its solubility in solvents of high polarity is strongly enhanced by the addition of >20 molar equivalents of strong acid. The titration of these species with hydrochloric acid suggests a complicated reaction equilibrium, perhaps involving several complex ions. Two additional terbium(III)-centered species' synthesis was attempted utilizing dmphen (= 2,9-dimethyl-1,10-phenathroline), and HdmphenCl (= 2,9-dimethyl1,10-phenathroline hydrochloride) as the ligands yielded a non-luminescent product. Elemental analysis, NMR spectroscopy, and single-crystal X-ray diffraction confirmed that the ligand is not directly bound to the metal center. Although this limits these product's utility as a sensing agent, it sheds light on the geometric constraints of ligand binding, and the distance limitations of the antenna effect.

Biography:

Justin Stace is an associate professor of chemistry at Belmont University, located in Nashville, Tennessee. He teaches undergraduate chemistry courses and directs a modest research project introducing students to the excitement and frustration of novel research focused on the photophysics and chemical reactivity of f-block metal-centered complexes.

Semiconductor to Topological Insulator Transition in Transition Metal Dichalcogenides Core-Shell Lateral Heterostructures

Pengpeng Zhang

Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan

Abstract

Polymorphic phase transition is an important route for engineering the properties of twodimensional materials. Heterostructure construction, on the other hand, not only allows the integration of different functionalities for device applications, but also enables the exploration of new physics arising from proximity coupling. Yet, implementing a design

that incorporates the advantages of both remains underexplored. In light of integrating heterostructure formation and phase engineering in one step, we demonstrate a novel phase transition technique based on the construction of lateral (WSe2/SnSe2) core-shell architecture by molecular beam epitaxy.1 A semiconductor to topological insulator (TI) transition associated with the polymorphic change of WSe2 core is revealed by scanning tunneling microscopy/ spectroscopy in conjunction with firstprinciples calculations. Since the proposed phase transition mechanism only fundamentally requires a van der Waals interacting substrate and sufficient core-shell lattice mismatch, the approach could be potentially versatile towards other transition metal dichalcogenides and vapor deposition methods. Reference: 1. Dong, X.; Lai, W.; Zhang, P. P., Semiconductor to Topological Insulator Transition Induced by Stress Propagation in Metal Dichalcogenide Core-Shell Lateral Heterostructures. Materials Horizons 8, 1029 (2021).

Biography:

Pengpeng Zhang is an associate professor in the Department of Physics and Astronomy at Michigan State University. Her research interests include low-dimensional materials, atomic processes in thin film growth, interfacial electronic structures, molecular self-assembly, and scanning probe microscopy.

Film formation on Mg alloy surface by multifunction cavitation using phosphoric acid

Masataka Ijiri

Tokyo Metropolitan University, Japan

Abstract

Magnesium (Mg) has the lowest standard electrode potential among practical metals and is chemically active, so it is easily corroded. Recently, anodizing and chemical conversion have been used as Mg surface treatments. This generally involves the use of phosphoric acid, in order to reduce environmental hazards. However, there are still problems such as low durability, high cost, and low strength of the films produced using phosphoric acid. There is currently no coating technology using phosphoric acid alone. In the present study, we investigated film formation to improve the corrosion resistance of Mg alloy based on multifunction cavitation involving ultrasonic irradiation and a water jet.

Biography:

Masataka Ijiri obtained a bachelor's degree in engineering, a Master's Degree in mechanical and systems engineering, and a Ph.D. Degree in engineering at Okayama University. He is a specialist in materials engineering for titanium alloys. After obtaining a doctoral degree, he was a postdoctoral researcher at Sanyo-Onoda city University and studied cavitation processing technology. Currently he is working as an assistant professor at the Department of Mechanical Systems Engineering, Tokyo Metropolitan University.

Tailor-made synthesis of metal and metal oxide nanocrystals via thermal decomposition self-reducible metal complex in a small amount alkylamine mixture.

Takanari Togashi*

Yamagata University, Japan

Abstract

Inorganic nanoparticles, such as metal and metal oxide nanoparticle, are among the most studied materials in nanoscience because of their dispersibility in solvents and their unique optical, magnetic, catalytic, and electronic properties. These properties strongly depend on the shape and size of nanoparticles. Therefore, the size tunable synthesis of inorganic with narrow size distribution is fundamental for the advancement of nanoparticle technology in fields ranging from catalysts to electronics, energy conversion, and medicine. Size of inorganic nanoparticle have been controlled by tuning pf reaction parameters such as temperature, reacntion time and the amount of precursor and surfactant in solution media with low concentrations of metal precursors, leading to the production of large amounts of wastes. This has considerable environmental implications from view point of green chemistry, render the methods unfavorable for practical use. Here, the size tunable synthesis of inorganic nanoparticle via thermal decomposition of metal oxalate in small amount of alkylamine mixture keeping constant reaction volume using theoretical approach based on the LaMer model will be shown. The particle size of can be predicted from size of seed crystal and the amount of metal oxalate. Removal of the counter ion will be new concept for predictable size tuning of inorganic nanoparticle in highly concentrated solution.

Biography:

Takanari Togashi is an Associate Professor of Faculty of Science, Yamagata University. He received his BSc and MSc in Materials and Biological Chemistry from Yamagata University, followed by PhD in Chemical Engineering from Tohoku University, Japan.

Atomic force microscope-based study on the 0D and 2D nanomaterials

Sangmin An*

Department of Physics, Institute of Photonics and Information Technology, Jeonbuk National University, Jeonju 54896, South Korea

Abstract

Nanoscale water plays crucial role in biological system, lubrication system, even in atmospheric environment [1,2]. However, it is difficult to investigate its mechanical properties due to technical difficulty of well-defined shape of nanoscale water singlet. Here, I show how to form a nanoscale water meniscus in ambient conditions and investigate its mechanical properties by using a quartz tuning forkbased atomic force microscopy (QTF-AFM) [3]. In addition, I show the atomic force microscope-based 2D study via a Young's modulus imaging [4], Kelvin probe force microscopy (KPFM) including friction measurement.

Biography:

Sangmin An is the assistant professor in Department of Physics of Jeonbuk National University (Korea). He received PhD in Physics (AFM-based research) from Seoul National University (Korea) in 2013. Following AFM research in the National Institute of Standard and Technology

(NIST), USA for 3 years, he studied the nanoscale soft matter physics via a specialized AFM in SNU as a research assistant professor for 3 years. Currently, he is focusing on the 0D (Quantum dot) or 2D (Graphene, TMD) nanomaterials by using the advanced AFM, STM, SEM.

Effect of Imidazole as Corrosion Inhibitor on Carbon Steel Weldment in District Heating Water

Sang-Jin Ko[1]
Seok-Ryul Choi[1]
Min-Sung Hong[1]
Woo-Cheol Kim[2]
Jung-Gu Kim[1*]

[1]School of Advanced Materials Science and Engineering, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon 16419, Korea.

[2]Technical Efficiency Research Team, Korea District Heating Corporation, 92 Gigok-ro, Yongin 06340, Korea.

Abstract

Many research studies have been conducted on the corrosion inhibition performance of imidazole in acidic environments such as in the piping of a petrochemical plant. However, there has been no study on the effect of imidazole in alkaline conditions such as a local district water heating environment. Therefore, in this study, the effect of imidazole as a corrosion inhibitor on carbon steel weldment was investigated in alkaline district heating water. Inhibition efficiency and electrochemical properties were investigated by potentiodynamic polarization test and electrochemical impedance spectroscopy. As the concentration of imidazole increased up to 500 ppm, inhibition efficiency increased up to 91.7%. At 1000 ppm, inhibition efficiency decreased. Atomic force microscopy showed that surface coverage of imidazole at 1000 ppm is lower than that of imidazole at 500 ppm. X-ray photoelectron spectroscopy showed that with 500 ppm of imidazole, the amount of pyrrole type interaction is 4.8 times larger than pyridine type interaction. At 1000 ppm of imidazole, the amount of pyridine type interaction is 3.49 times larger than pyrrole type interaction. Depending on the concentration of imidazole, the ratio of interaction between carbon steel and imidazole affected inhibition efficiency.

Control of Nanostructures through Self-assembly of Kaolinite Nanoplatelets

JingChang [1,2*]
Bo Liu [2,3]
Zhen Li[1]
Qingxia Liu [2,4]
Zhenghe Xu [2,5]

[1]Xi'an University of Science and Technology, China

[2]University of Alberta, Canada

[3]East China University of Science and Technology, China

[4]Shenzhen Technology University, China 5Southern University of Science and Technology, China

Abstract

Hypothesis: The self-assembly of platy clay particles is influenced by anisotropic surface

chargingproperties of the particles. The Stern potentials of particle surfaces are controlled by electrolytetype, electrolyte concentration and solution pH. Consequently, the energy-favorable particle associationvaries with solution condition, leading to different self-assembly structures. Therefore, it shouldbepossible to form desired nanostructure of final clay product through self-assembly of clay particles bycontrolling the surface charge through adjusting solution condition. Experiments: Atomic force microscopy (AFM) was used to image in liquids the surface lattice structureof two kaolinite basal planes in the presence and absence of monovalent cations to identify theionadsorption mechanisms. Based on the understanding of ions adsorption mechanisms atkaolinite−aqueous interfaces, three different surfaces of kaolinite nanoparticles were selectivelyexposed for Stern potential determination using AFM. Aggregation structures through particleself- assembly were predicted by analyzing the interaction energies between various types of surfaces of kaolinite particles. The structures were visually confirmed using the freeze-dried scanning electronmicroscopy technique. Findings: In a 10 mM KCl solution, by reducing pH of a concentrated kaolinite suspension from8 to5and3, the dispersed particles were self-assembled to a well-stacked configuration and card-house structure, respectively. Current study demonstrates that surface charging properties of platy kaolinitenanoparticles can be successfully used to understand the rheology behavior of kaolinite nanoparticlesuspensions and design nanostructures of clay products (catalysts and sorbents). The self-assemblyisalso applicable to other platy particles of anisotropic surface properties.

Biography:

Jing Chang is an assistant professor in Xi'an University of Science and Technology. Dr. Chang's research interests are in colloid and surface science, nanotechnology, and advancedfunctional materials, with a special focus on interfacial science and surface chemistry as applied to natural resources processing (such as minerals, oil sands, coal, petroleum, etc.) andutilization. Dr. Chang received her PhD degree in Chemical Engineering from University of Alberta(Supervisor: Dr. Zhenghe Xu, co-supervisor: Dr. Qingxia Liu) in 2019.

A brief introduction on computational materials science and its application in optoelectronic materials

Liujiang Zhou*

School of Physics, University of Electronic Science and Technology of China, Country

Abstract

Optoelectronic materials are the cornerstone of the photoelectric information fusion technology. Currently, the computational and data-driven sciences have become the main research paradigms in materials science. Computer design and performance simulation of optoelectronic materials at the atomic and molecular levels, which is supported by density functional theory (DFT) and post-DFT methods, play an important role in leading and promoting the research of optoelectronic technology. Based on the above theory and technology, in the past few years, we have built a framework for the design of optoelectronic material that have been successfully applied to the explorations of 2D/3D optoelectronic materials. Our research provides a theoretical basis for the development of a new generation of optoelectronic devices.

Biography:

Liujiang Zhou received his Ph.D. degree in 2014 from University of Chinese Academy of Sciences and performed postdoctoral research at University of Bremen, Germany (2014 2016) and at Los Alamos National Laboratory, USA (2017-2019). He started his own independent academic career as a professor at University of Electronic Science and Technology of China (2019). His research efforts are focused on optoelectronic information and energy materials, using a broad ranges of computational modeling techniques.

Modulating the Verwey transition and anomalous Hall effect of epitaxial Fe3O4 thin films by ionic gating

Quan-Lin Ye*

Hangzhou Key Laboratory of Quantum Matter, School of Physics, Hangzhou Normal University, Hangzhou 311121, China

Abstract

Understanding the Verwey transition in magnetite (Fe3O4), a strongly correlated magnetic oxide, is a one-century-old topic that recaptures great attention because of the recent spectroscopy studies revealing its orbital details. In this talk, we'll report our recent progress on the modulation of the Verwey transition by tuning the orbital configurations with ionic gating.1 In epitaxial magnetite thin films, the insulating Verwey state can be tuned continuously to be metallic showing that the low-temperature trimeron states can be controllably metalized by both the gate-induced oxygen vacancies and proton doping. The ionic gating can also reverse the sign of the anomalous Hall coefficient, indicating that the metallization is associated with the presence of a new type of carrier with competing spin. The variable spin orientation associated with the sign reversal is originated from the structural distortions driven by the gate-induced oxygen vacancies.

Biography:

Quan-Lin Ye is a professor of physics at Hangzhou Normal University (HZNU). Prior to joining HZNU, he spent more than 5 years as a postdoctoral researcher in Nagoya University and Nanyang Technological University. He was awarded the JSPS postdoctoral fellowship in 2007 and was a visiting scholar with University of Groningen from 2019-2020. Prof. Ye has been conducting research in the field of magnetic thin films and nanomaterials for over 20 years. His research interests include nanomaterials fabrication, electrical and magneto-transport, ionic gating, magnetic skyrmion, Mie scattering.

Potential use of spent abrasive waste as sustainable construction materials

Nor Hasanah Abdul Shukor Lim[1*]
Nur Balqis Idayu Mahmad Raseh[1]
Nur Farhayu Ariffin[2]
Mostafa Samadi[1]
Abdul Rahman Mohd Sam[1]

[1]Universiti Teknologi Malaysia, Malaysia,

[2]Universiti Malaysia Pahang, Malaysia

Abstract

The depletion of natural resources such as aggregates and the concern on the emission of carbon dioxide to the atmosphere have created interest in finding solution to the problem.

Besides, Malaysia imports huge amount of copper slag and garnet to be used as abrasive material for ship clearing and repairing, and resulting in spent copper slag and spent garnet as waste material. It has been estimated that 2,000 million tonnes of abrasive waste needs to be disposed annually. Therefore, this research investigates the potential of spent abrasive waste to be used in concrete. This research tends to investigate the suitability of spent copper slag as pozzolanic materials and the surface bonding between spent garnet with the binder. Various tests were carried out to determine the characteristic of materials including strength activity index, bulk density, sieve analysis and water absorption. For mechanical properties, compressive strength, flexural strength and splitting tensile strength were tested. 100% spent garnet replacement revealed the best performance in the engineering properties of concrete. In addition, the use of 20% of spent copper slag as cement replacement produced higher compressive strength at the age of 28 days by 14% compared with control specimens. The results revealed that spent garnet and spent copper slag can be used as cement and fine aggregates replacement in concrete production as the it improve the properties of concrete. In addition, the environmental impact can also be reduced through the use of spent abrasive waste by preserving the use of natural resources.

Biography:

Nor Hasanah is a senior lecturer in Universiti Teknologi Malaysia and a registered professional Technologist under Malaysian Board of Technologist. Her research interests can be broadly categorized into four primary areas of specialization; Green materials in construction buildings; Nanomaterials; Geopolymer and Sustainable waste materials. She has developed number of award winning research products that have been patented and trademarked in Malaysian construction industry. She has published more than 50 publications in peer review journals with h-index 15. She is a dedicated team member as well as a team leader with intending attention to support diversity in global scientific communities.

Enhancement of Mechanical Properties of Ti-6Al-4V through High-Density Pulsed Electric-Current

Rui Iwase
Shaojie Gu
Yasuhiro Kimura
Yuhki Toku
Yang Ju*

Department of Micro-Nano Mechanical Science and Engineering, Graduate school of Engineering, Nagoya University, Nagoya 464-8603, Japan

Abstract

As a versatile material, titanium alloy has been widely used in many places such as aircraft parts, steam turbines, automotive engines, and medical devices, etc. Normally, hot working and heat treatment are necessary in the manufacturing process of titanium alloy in order to improve its processability due to the relative low ductility of the material at room temperature. Recently, we have proposed a new method to improve the mechanical properties of metallic materials based on the treatment of high-density pulsed electric-current (HDPEC). It has been studied as a state of art method to repair damage and to enhance fatigue life of metallic materials. This study focuses on the investigation of the effect of HDPEC on the mechanical properties of dual-phase α/β titanium alloy Ti-6Al-4V. Material characterization shows that the

grain refinement was achieved after HDPEC treatment, resulting in strengthening in Ti-6Al-4V. In addition, it was found that the phase transformation from α-Ti to β-Ti was induced after HDPEC treatment. The improved β-Ti phase contributes to the increase of ductility since β-Ti possesses better ductility than α-Ti. Therefore, this novel method could be used to modify the microstructure and thereby enhanceing the mechanical properties of dual-phase α/β titanium alloys.

Biography:

Yang Ju received a B. Eng. in 1985 and a Ms. Eng. in 1991 in Electrical Engineering from Shandong University of Technology and Tsinghua University, China, respectively. He received a Dr. Eng. in 1999 in Mechanical Engineering from Tohoku University, Japan. He became an associate professor in 2003 at Tohoku University, and a professor in 2007 at Nagoya University, Japan. Professor Ju's research interests include damage recovery, crack healing and property enhancement of metallic materials; creation and development of functional nano and bio materials. He has published more than 200 manuscripts in Archival Journals, and has 16 patents in Japan and United States. Prof. Ju received The Japan Society of Mechanical Engineers Medal in 2006. He became a Fellow of The Japan Society of Mechanical Engineers in 2018, and a member of The Engineering Academy of Japan in 2021.

Notch effect and thickness effect on the stress triaxiality behavior and fracture mechanisms of Al alloy specimens

Liang Wang[1*]
Xiao Du[1]
Nak-Sam Choi[2]

[1]Department of Mechanical Design Engineering, Graduate School, Hanyang University, Seoul, Korea

[2]Department of Mechanical Engineering, Hanyang University, Ansan, Gyeonggi-do, Korea.

Abstract

In Al alloy, various stress triaxiality behaviors are formed according to the notch radius and specimen thickness. In this study, the stress triaxiality behaviors at four representative sites were interpreted by combining the DIC and FEM. The fracture surface was observed using the SEM. For small notched specimens, the maximum stress triaxiality at the internal site increases with increasing thickness. With an increase in the thickness, the shear fracture behavior changesfrom the out-of-plane shear to the in-plane shear, and the fracture behavior changes from the shear mode to the tensile-shear mixed fracture mode.

Biography:

Liang Wang is working at the Department of Mechanical Design Engineering, Graduate School, Hanyang University, Korea. His research area is composite analysis and material design.

Tailoring liquid-vapor condensation phenomena: challenges and opportunities

Youngsuk Nam

Korea Advanced Institute of Science and Technology, South Korea

Abstract

Liquid-vapor condensation is a ubiquitous phase change process that is essential in both nature and industry. The enhancement of heat and mass transfer during condensation can provide substantial economic and environmental benefits to various applications, including power generation, thermal management, water management, refrigeration, and environmental conditioning. Previous studies showed that the coalescence-induced droplet jumping phenomena substantially enhanced the condensation heat transfer by facilitating droplet removal and surface refreshment. However, applying such condensers to real-world applications has been restricted by several challenges. Most importantly, their performance rapidly decreased at a high supersaturation level due to the flooding. Second, typical low surface energy coatings applied to such condensers showed limited thermal stability; therefore, the performance rapidly decreased in a hot steam environment. Finally, the droplet jumping condensers could not provide the enhanced heat transfer for low surface tension fluids such as alcohols and refrigerants. In this talk, we will summarize our efforts to overcome such challenges. We will discuss the flooding mechanism by suggesting anti-flooding strategies. We will also introduce scalable inorganic condensers with excellent thermal stability and lubricant-infused condensers with enhanced heat transfer and long-term stability. Later in the talk, we will briefly discuss other potential opportunities associated with tailoring condensation phenomena.

End of Day 05 Parallel Session II

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8105, Rasor Blvd - Suite #112, PLANO, TX 75024

Tel: +1-469-854-2280/81; **Fax:** +1-469-854-2278; **Toll free:** +1-844-395-4102;

Email: materials@uniscigroup.net (or) business@matscienceconference.com

Web: https://www.matscienceconference.com/