



11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Scientific Tracks & Abstracts Day 1

Advanced Materials 2017

## Advancement in Nanomaterials Science And Nanotechnology | Coatings and Surface Engineering | Functional Materials

### Session Chair

**Hideo Miura**

Tohoku University, Japan

### Session Chair

**Manfred Martin**

RWTH Aachen University, Germany

### Session Introduction

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**Title: TiO<sub>2</sub> nanotubes as potential vascular stents: Effect of oxygen plasma treatment on crystal structure and surface properties**

**Metka bencina**, Jožef Stefan Institute, Slovenia

**Title: Particle size versus energetics of nanomaterials: Key parameters controlling the stability and reactivity of nanostructured materials**

**Speranta Tanasescu**, Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, Romania

**Title: Formation of carbon-based nanostructures from carbon suboxide decomposition at high pressure and temperature – A ReaxFF study**

**Xavier bidault**, Commissariat Energie Atomique, France

**Title: Starch capped silver nanoparticles as colorimetric sensor for hydrogen peroxide recognition in aqueous medium**

**Abdelaziz Elgamouz**, University of Sharjah, UAE

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# ADVANCED MATERIALS & PROCESSING

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## Evaluation of atomic scale damages of advanced materials based on the order of atom arrangement

**Hideo Miura**

Tohoku University, Japan

Recently, mechanical properties of polycrystalline materials have been found to vary drastically depending on their micro texture. The crystallinity of grain boundaries was found to dominate both their mechanical and electrical properties and the long-term reliability. This is because various defects such as strain, vacancies, impurities, and dislocations easily concentrate around grain boundaries and thus, degrade the quality of atomic configuration in grains and grain boundaries. In this talk, a grain boundary is defined by volumetric transition area between two grains, though it has been defined as a line interface between nearby grains. The quality of grain boundaries is independent of crystallographic orientation of nearby grains. The diffusion of component elements is remarkably dominated by the local quality of grain boundaries. The degradation of materials mainly starts to occur around grain boundaries with low crystallinity and atomic diffusion, such as strain-induced anisotropic diffusion and electro migration, is accelerated drastically along the poor-quality grain boundaries. The initial micro texture of various heat-resistant alloys has been found to degrade under operating conditions of advanced high efficient thermal power plants based on this strain-induced accelerated diffusion of component elements. The quality of thin-film interconnections in advanced semiconductor devices has been decreased under operation by electro- and stress-induced migration of component elements. Therefore, it is very important to evaluate the crystallinity of advanced materials quantitatively for assuring safe and reliable operation of various products. Crystallinity of grain boundaries can be evaluated quantitatively by applying electron back-scatter diffraction (EBSD) method. The order of atomic alignment in the observed area is analyzed by the sharpness of Kikuchi lines obtained from the observed area. Various materials properties vary drastically depending on the order of atomic alignment, in particular, in grain boundaries. Both fluctuation and degradation of various properties of materials such as heat-resistant alloys and thin films are investigated from the viewpoint of the crystallinity of grains and grain boundaries.

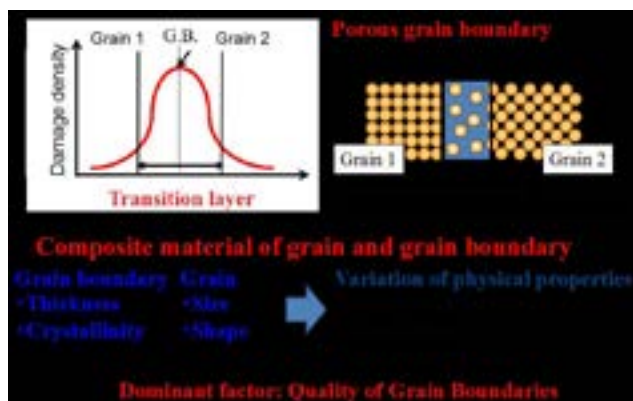


Figure1: Variation of crystallographic quality (order of atom arrangement) of a grain boundary

### Biography

Prof. Hideo Miura has received his PhD from Tohoku University, Japan. He had worked for Hitachi Ltd., Japan for 20 years as a Chief Researcher of mechanical reliability of various products and moved to Tohoku University in 2003. He is the director and Professor of Fracture and Reliability Research Institute. His main research topic now is prediction and prevention of fracture of advanced functional materials and thin-film devices. He has published more than 200 technical papers in the field of mechanical reliability of various materials and thin-film devices, and obtained more than 200 patents all over the world. He also has been serving as an organizer of various international conferences.

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## Thermokinetic modeling and simulation of complex phase transformations in the framework of advanced functional materials

**Erwin Povoden-Karadeniz**

TU Wien, Institute of Materials Science and Technology, Austria

At present, computational materials engineering is a desired and propagated aim of academia and industry. The usability of computational thermodynamics for physically-based simulations of materials behaviour during technological processing and applications requires a step ahead of classical equilibrium thermodynamic phase descriptions. Theoretic requirements for successful predictions of complex phase evolutions during technological treatments, and related relevant properties, are discussed for two selective, promising functional materials groups. The principles of defect modelling and associated efficiency calculations of complex catalytic materials are discussed for multicomponent nonstoichiometric rare-earth based perovskite oxides. In the functional metals field, simulations of thermo kinetic evolution of metastable precipitates in Ti-Ni based shape memory alloys as function of thermo-mechanical processing is presented. Potentials and limitations of integrated thermo kinetic simulations of phase transformations are highlighted.

### Biography

Dr. Erwin Povoden-Karadeniz is an assistant professor at TU Wien, Institute of Materials Science and Technology, Austria at present. His international experience includes various programs, contributions and participation in different countries for diverse fields of study. His research interests as a Scientist reflect in his wide range of publications in various national and international journals.

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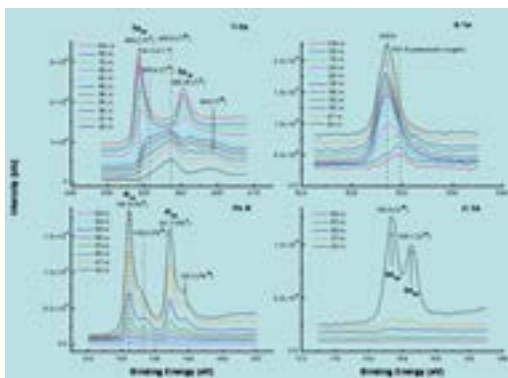
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## Evaluation of sputtered PZT thin films on Ti-substrates upon re-crystallization with a thin Pb-overcoat

**Ankita Ghatak**

S.N. Bose National Centre For Basic Sciences, India

Processing of thin lead zirconate titanate (PZT) films on metallic substrates has several advantages such as high frequency operation, low electrical series resistance, low dielectric loss and potential for embedded capacitor systems. As a suitable metal support for PZT films, titanium (Ti) seems to be the most natural choice as it possess high melting point, the thermal expansion coefficient of Ti matches closely to that of PZT and permits good adhesion with low reactivity. However, ferroelectric and piezoelectric responses of PZT films on Ti substrates are found to be not that encouraging. Presence of a non-ferroelectric pyrochlore/ fluorite (Py/FI) phase on the surface of the PZT film is believed to be the primary cause for poor electrical performance. In this work, effect of re-crystallization of PZT films with a thin Pb-overcoat has been investigated through structural, morphological, compositional and electrical studies. Sputter deposited PZT thin films on Ti-substrates are found to contain a Pb-deficient and Zr-enriched Py/FI phase of type  $Pb_2(Zr,Ti)_2O_6$  on the surface of the PZT film. Re-crystallization of these PZT films with a thin lead (Pb) overcoat improves the degree of crystallization, morphology and dielectric/ Ferroelectric properties of the films by converting the top Pb-lean and Zr-rich Py/FI phase into perovskite phase. Structural changes that occur in PZT films upon re-crystallization with a Pb-overcoat have been correlated with ferroelectric characteristics of the PZT films.



### Biography

Ankita Ghatak, National Postdoctoral Fellow has her expertise in growth of nanostructured binary as well as complex oxides. She has grown aligned 1-D nanostructured binary oxide which has a strong influence in the field of applications. She has hands on expertise on microstructural analysis of complex oxide nanostructures that has provided up a new field of research from technological point of view. Her interface analysis of complex materials with substrates has open up a challenging field in the device fabrication process. She in her publications has tremendously contributed about the benefit of creating atomically sharp interfaces that will enhance the future device performances. A new approach in looking into atomic columns of manganite nanowires has been achieved by her recently through structural simulation.

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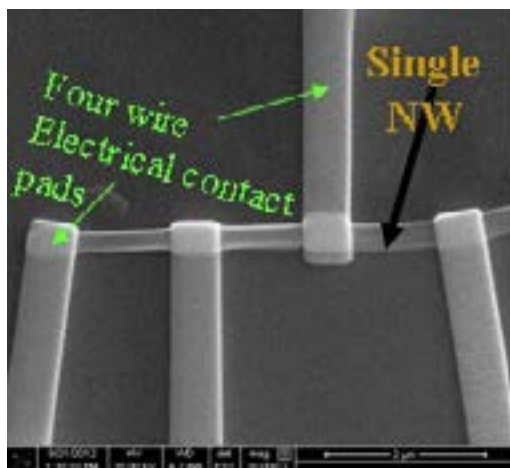
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## Modification of ground state property on size reduction to 1D

**Barnali Ghosh**

S.N. Bose National Centre for Basic Sciences, India

Nanowires, because of their unique one-dimensional like structural characteristics and size effects, exhibit many novel physical properties, that are different from their bulk counterparts. Main motivation of our investigation is to show, how size reduction affects competing interactions in complex oxides and thus, changes their ground state. Magnetization measurement on half doped manganite nanowire shows several magnetic transitions which are different from bulk. Understanding of magnetic transitions done using several experiments like magneto caloric study, Neutron diffraction study, which shows the presence of phase coexistence of magnetic phases (antiferromagnetic and ferromagnetic). As the experiments are carried out on ensemble of nanowires, question may arise whether the phase coexistence observed in nanowires is due to size dispersion. To answer this question, instead of ensemble of nanowires, noise spectroscopy study of single nanowire (<50 nm) level is done to demonstrate how the noise spectroscopy can explain the magnetic transitions and phase separation. Field dependent as well as temperature dependent noise spectroscopy study was done on a single nano-wire to avoid the problems of size dispersion with the specific aim of corroborating the magnetic phase transitions as well as phase co-existence at a single NW level. I would discuss briefly on how to grow nano structured material and about the experiments both in ensemble and single nanowire of perovskite oxides. Experiments with single nanowires; mainly on fabrication of single nanowire based devices, using different lithographic techniques challenges would be discussed.



### Biography

Dr. Barnali Ghosh (Saha), is now a Scientist-E, (Associate Professor) in the Department of Condensed Matter Physics and Material Sciences and Head of the department of Technical Research facility programme. She is a member of Indian Physics Association. She got Ph.D degree in Physic award in 1998. She got a research Award in Woman Scientist programme in 2003 and 2008 from "Department of Science and Technology, Government of India". Currently Dr. Barnali Ghosh (Saha)'s researches focus on experimental condensed matter Physics and Nano Science and nanotechnology, Physics of transition metal oxides mainly perovskite oxides. She is also working on fabrication of single nanowire based devices using different lithographic techniques like, e-beam and focused ion beam techniques and transport measurement on single nanowire. She also does cross sectional transmission electron microscopy relate work using focused ion beam based techniques.

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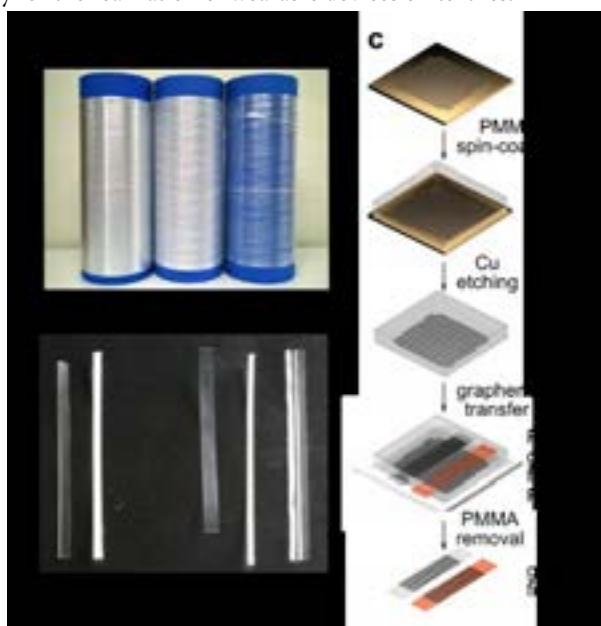
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## Towards conductive textiles: Coating polymeric fibers with graphene

Ana I. S. Neves<sup>1</sup>, Elias Torres Alonso<sup>1</sup>, Saverio Russo<sup>1</sup>, Monica F. Craciun<sup>1</sup>, Daniela P. Rodrigues<sup>2</sup> and Helena Alves<sup>2</sup><sup>1</sup>University of Exeter, UK<sup>2</sup>University of Aveiro, Portugal

The concept of smart-textiles is witnessing a rapid development with recent advances in nanotechnology and materials engineering. Bearing in mind that the concept of textiles is much wider than clothes and garments, the potential is immense. While most current commercial applications rely on conventional hardware simply mounted onto fibers or fabrics, a new approach to e-textiles consisting in using functionalized textiles for several technological applications has the potential to change the paradigm of wearable electronics completely. Conducting fibers are an important component of any e-textile, not only because they can be used as wiring for simple textile-based electronic component, but also because they can be used to build electronic devices directly on textile fibers. We have reported a new method to coat insulating textile fibers with Monolayer graphene to make them conductive while preserving their appearance. There are a number of factors that can greatly influence the sheet resistance achieved by graphene-coated textile fibers. In order to understand the influence of the topography of the fibers on the effectiveness of the graphene coating, an extensive study encompassing microscopy techniques like Atomic Force Microscopy and Scanning Thermal Microscopy, as well as Raman spectroscopy was performed. This method has proven to be a versatile tool to achieve flexible, transparent and conducting fibers of different materials, sizes and shapes. The first applications of electronic devices built on such fibers are demonstrated, with an alternating current electroluminescent device, following previous work in our group on similar devices in flexible substrates. This opens up the way for the realization of wearable devices on textiles.



**Figure 1:** a) Photo of the fibres in reels. b) Photo of the fibres cut to ca. 3 cm length. c) Schematic representation of the graphene transfer onto textile fibres

### Biography

Dr Ana Neves has a background in Chemistry, with a PhD awarded by IST, University of Lisbon, Portugal, for work carried out at the Solid State Group of ITN (Lisbon), on the molecular engineering of materials with magnetic and electric properties. Pursuing the path of applications, she joined the Organic Electronics group at INESC –Microsystems and Nanotechnology in Lisbon in 2013 as a postdoctoral researcher. Dr Neves joined the University of Exeter in October 2014 as an Associate Research Fellow under the project "Wearable light emitting transistors for future communication devices". Since October 2016 she is a Lecturer in Engineering, and currently holds a Marie Skłodowska-Curie Individual Fellowship with project E-TEX "All-organic devices in textiles for wearable electronics". She is also a member of the Nano-Engineering, Science and Technology Group (NEST).

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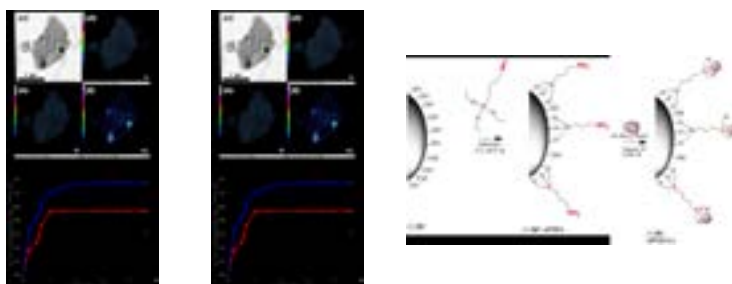
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## Functionalization of cocoa shell (CS) surfaces using nanoparticles and their application in CO<sub>2</sub> storage

**Julien Vieillard**

Université de Rouen Normandie, France

The aim of this research is to investigate how the covalent grafting of cocoa shell surface (CS) may improve its activity for the adsorption of CO<sub>2</sub> at 20°C. Pure cocoa shells (CS) are agricultural by-products, usually inexpensive and abundantly available. They were functionalized by salinization and subsequent immobilization of cobalt nanoparticles (Co-NPs). In parallel, some carbon material was generated by hydrothermal treatment then post functionalized to increase the cocoa shell specific surface. Finally some core-shell nanoparticles have been also synthesized using cocoa shell as a core and zinc oxide as a shell, then some post-functionalization with nanoparticles insertion were added. The physical and thermal properties of the adsorbents like analysis stability, surface charge and morphology were investigated by FTIR, SEM, TEM, EDX, BET, DSC and zeta potentiometry techniques. The performance for the CO<sub>2</sub> capture was investigated and the high adsorption capacity was mainly attributed to their original structure.



### Biography

Julien Vieillard has his expertise in analytical chemistry in order to promote innovative material or new application. Thus, in the recent year, we tried to promote natural bio waste for CO<sub>2</sub> sorption. Actually, our research is also focused to develop original optical, electrochemical biosensors and antibacterial treatment for metallic surface.

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## Low friction, wear resistant quasicrystalline coatings

**Jean-Marie Dubois**University de Lorraine, France  
Jozef Stefan Institute, Slovenia

Quasicrystals were discovered in 1982 by Shechtman, Nobel Prize in Chemistry 2011, and have since been the focus of intense research regarding their atomic structure, their properties and potential usefulness. Among the few niches of application that were sorted out so far is the possibility to use them as a low friction counterpart in mechanical devices. Typical friction coefficients pointed out against hard steel is indeed about half that observed with conventional metallic metals or with hard steel sliding against itself. Wear during short pin-on-disk tests is also very much reduced. The intrinsic brittleness of quasicrystals is however very much detrimental to such an application, which could not be implemented on realistic devices. We came however to a totally different issue in recent years when we could show that an appropriately prepared quasicrystalline coating can produce friction as low as 6% against hard steel and sintered tungsten carbide whereas wear is negligible for extremely long pin-on-disk tests (i.e. lasting for at least 5 km), see left hand side of the image. The talk will summarize our findings in this area and show how low friction is related to the specific electronic structure of quasicrystals, which determines their surface energy. An overview on other characteristic application niches of quasicrystals will be given.

### Biography

Jean-Marie Dubois is a director of research emeritus at CNRS, France and a part time scientific adviser at Jozef Stefan Institute in Ljubljana, Slovenia. He has dedicated a large fraction of his research efforts to promoting specific applications of quasicrystalline materials (tribology, adhesion, heat insulation) in parallel to his fundamental studies of the atomic structure, electronic structure and electron transport properties of this new type of aperiodic matter.

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## Hafnium and palladium modified aluminide coatings

Jolanta Romanowska and Maryana Zagula-Yavorska  
Rzeszów University of Technology, Poland

Hafnium or palladium modification of NiAl phase increases the oxidation resistance of aluminide coatings deposited on turbine blades in a hot section of jet engines. Small hafnium or palladium addition to aluminide coatings decreases the oxidation rate of turbine blades made of nickel superalloys. Small content of hafnium (0.1-1.0 % wt) improves high temperature mechanical properties of aluminized nickel based superalloys. Palladium modification increased the outer zone hardness. It is due to the presence of the  $\sigma$  and  $\mu$  phases. The palladium or hafnium modified aluminide coatings have better oxidation resistance than the non-modified ones. The use of 'co-doping' has recently been emphasized as a strategy for optimizing the oxidation resistance of superalloys, conventional alloys and coatings. The comparison of structures of hafnium and palladium modified aluminide coatings deposited on pure nickel and CMSX<sub>4</sub> nickel superalloy is presented. Aluminide layers were deposited by the Chemical vapor deposition (CVD) method. Hafnium was deposited simultaneously with aluminum. Aluminum was deposited from the AlCl<sub>3</sub> and hafnium from the HfCl<sub>3</sub> gas phases. Palladium was deposited by the electrodeposition method. The obtained coatings were examined using an optical microscope, a scanning electron microscope and an XRD phase analyzer. Both coatings consist of two layers; an outer, comprising the  $\beta$ -NiAl phase and the interdiffusion one. The interdiffusion layer on pure nickel consists of the  $\gamma'$ -Ni<sub>3</sub>Al phase, whereas on the CMSX<sub>4</sub> – of the  $\beta$ -NiAl phase. Small inclusions of Pd and Hf rich phases were found at the border of the layers on nickel, whereas inclusion containing Pd, Hf and refractory elements were observed in the interdiffusion zone on the CMSX<sub>4</sub> superalloy. The research has been supported by the National Science Centre, Poland Grant No. 2015/19/B/ST8/01645.

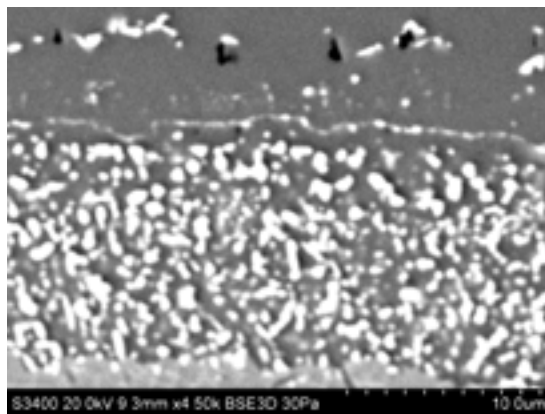


Fig.1: Cross-section microstructure of aluminide coating obtained by CVD method on pure nickel (a), and CMSX<sub>4</sub> nickel superalloy (b)

### Biography

Jolanta Romanowska has completed her PhD from AGH University of Science and Technology, Cracow, Poland and DSC from the Silesian University of Technology, Poland. She is the professor at the Rzeszów University of Technology, Poland. She has published more than 50 papers in reputed journals. She has her expertise in thermodynamics of alloys and protective coatings. She elaborated the model of predicting thermodynamic properties of ternary alloys on the basis of thermodynamic properties of binary alloys.

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## Resistive switching in highly disordered thin oxide films

Manfred Martin<sup>1</sup>, Yoshitaka Aoki<sup>1,2</sup>, Philipp Hein<sup>1</sup> and Alexandra von der Heiden<sup>1</sup><sup>1</sup>RWTH Aachen University, Germany<sup>2</sup>Hokkaido University, Japan

In thin films of mixed ionic electronic conductors sandwiched by two ion-blocking electrodes, the homogeneous migration of ions and their polarization will modify the electronic carrier distribution across the conductor, thereby enabling homogeneous resistive switching. Here we report non-filamentary memristive switching based on the bulk oxide ion conductivity of amorphous GaOx ( $x \sim 1.1$ ) thin films. We directly observe reversible enrichment and depletion of oxygen ions at the blocking electrodes responding to the bias polarity by using photoemission and transmission electron microscopies, proving that oxygen ion mobility causes memristive behavior. The shape of the Hysteresis I-V curves are tunable by the bias history, as found in the mathematically derived memristor model. This dynamical behavior can be attributed to the coupled ion drift and diffusion motion and the oxygen concentration profile acting as a state function of the memristor. Further examples will be discussed.

### Biography

Manfred Martin is Professor and Head of the Institute of Physical Chemistry of RWTH Aachen University, Germany. At Seoul National University, Korea he was WCU Professor and is now Adjunct Professor. He has more than 30 years of experience in education and research of physical chemistry of solids as well as service at department, faculty and university level. His current research focusses on materials for energy conversion, resistive switching, solid-state reactions, secondary ion mass spectrometry, and computer simulations as well. Professor Manfred Martin has published >200 scientific papers in international, refereed journals. He received the Carl-Wagner Award and has been elected as member of the Royal Society of Chemistry. He has supervised more than 50 Ph.D. students and more than 20 postdoctoral fellows.

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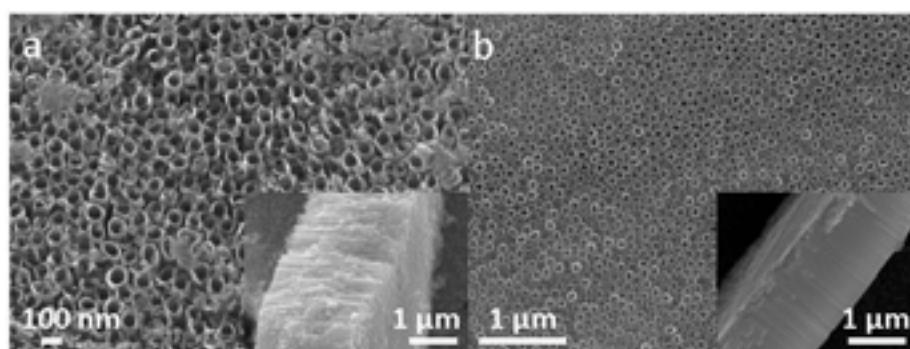
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September 07-08, 2017 | Edinburgh, Scotland

## TiO<sub>2</sub> nanotubes as potential vascular stents: effect of oxygen plasma treatment on crystal structure and surface properties

Metka Benčina<sup>1</sup>, Iva Junkar<sup>1</sup>, Tomaž Lampe<sup>2</sup>, Aleš Igljič<sup>2</sup>, Veronika Kralj-Igljič<sup>2</sup>, Matjaz Valant<sup>3</sup> and Mukta Kulkarni<sup>4</sup><sup>1</sup>Jožef Stefan Institute, Slovenia<sup>2</sup>University of Ljubljana, Slovenia<sup>3</sup>University of Nova Gorica, Slovenia<sup>4</sup>Palacky University, Czech Republic

Despite intensive research and applications of different techniques to improve surface properties of vascular stents, currently available metal stents and their coatings (*DES* - drug eluting stents) still lack of desired surface biocompatibility, mostly due to mechanical injuries, inflammation, as well as proliferation and migration of smooth muscle cells, often with progression to restenosis. Besides, the durability and stability of *DES* is still problematic and has been connected with high risk of thrombosis. Biomimetic nano-sized materials, with their crystal structure, surface morphology and chemical properties are one of critical features for their potential use in vascular stent applications, which should support adhesion, proliferation and differentiation of endothelial cells and prevent abnormal growth of smooth muscle cells. For example, it was shown that titanium dioxide (TiO<sub>2</sub>) nanotubes (NTs) topography is essential parameter in optimizing endothelial cell and smooth muscle cell responses to vascular implants. The purpose of this study is to investigate surface properties and crystal structure of TiO<sub>2</sub> NTs. Since the oxygen plasma treatment plays significant role in surface treatment of biomedical devices due to surface cleaning and sterilization, its effect on the mechanical stability and surface chemical properties was evaluated. Vertically aligned arrays of TiO<sub>2</sub> NTs were synthesized on Ti metallic substrates with electrochemical anodization. The crystal structure was investigated with X-ray Diffraction Spectroscopy, while morphology and surface properties were analyzed with Scanning Electron Microscopy coupled with Energy Dispersive X-ray Analysis, X-ray Photoelectron Spectroscopy and Water Contact Angle analysis. Our results indicate that oxygen plasma treatment of TiO<sub>2</sub> NTs surfaces induces the formation of oxide layer on the surface of TiO<sub>2</sub> NT, which could result in enhanced biocompatibility. Moreover, plasma treatment removes undesired electrolyte residues on TiO<sub>2</sub> NTs surface and highly improves its wettability. We showed that plasma treated TiO<sub>2</sub> NTs possess long-term hydrophilicity and influence on crystallization of amorphous TiO<sub>2</sub> NTs to anatase and/or rutile crystal phase, which could be the reason for improved wettability. The optimized conditions (power, frequency and time) of oxygen plasma treatment on the mechanical stability of TiO<sub>2</sub> NTs are also presented. Oxygen plasma treatment can greatly improve the surface characteristics of biomimetic materials and enhance their biocompatibility. Restenosis and thrombosis still remain a serious concern and should be given a great deal of attention in order to produce improved tissue-material response.



**Fig.1:** SEM images of TiO<sub>2</sub> NTs after plasma treatment at a.) non-optimized conditions; structure is destructed, NTs are partially closed and b.) optimized conditions; NTs are well defined, tops are open.

### Biography

Metka Benčina has her expertise in synthesis and characterization of nanomaterials for photocatalytic and biomedical applications. She produced novel metal oxides with pyrochlore structure and proved their absorption in visible range of EM spectrum and enhanced photocatalytic properties under UV and visible light irradiation. Currently she is fabricating TiO<sub>2</sub> nanostructural surfaces and investigating their applications in biomedicine - biosensors for detection and treatment of cancer cells, photo-assisted cancer treatment and biomimicking vascular stents. Her particular research interest is the effect of oxygen plasma treatment of biomaterials.

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## Particle size versus energetics of nanomaterials: Key parameters controlling the stability and reactivity of nanostructured materials

**Speranta Tanasescu**

Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, Romania

Due to the unique and unusual physical and chemical properties of the systems and structures at the nanoscale, the understanding of their stability and reactivity, presents a host of questions and problems. The dimension-dependent properties or phenomena may be used for functional effects, the nanotechnology taking advantage of this by designing property modifications for applicative reasons. At the same time, research to date suggests that some engineered nanomaterials will present hazards, thus challenging many conventional approaches related to nanosafety area. Because this is an emerging scientific issue, to identify key parameters important for evaluating the possible benefits as well as risks is a central point in the research activity with impact in the materials science. In the present paper will be argued that control of the energetic parameters and the understanding of their crossover when working at the nano-level are important steps in understanding the nanomaterial stability and the possibilities to interaction with the biologic systems. Some compounds from specific systems were selected for Discussion: nanostructured transition metal oxides; Nano alloys, bio-nonbio systems. Several conclusions can be drawn from the characterization data obtained so far: •Exploring the relationships between different compositional variables and thermodynamic properties of Nano crystalline transition metal oxides we obtained that particular behavior of these materials could be explained not only qualitatively by the structural changes, but also by the fact that the energetic properties are extremely sensitive to the chemical defects in oxygen sites. •Investigating the metastable phases of Nano alloys synthesized by severe deformation non-equilibrium methods we obtained that the energetic parameters may be used to explain the experimentally observed stability in particular temperature ranges associated with the growth process of nanometer-sized samples. •The evaluation of the thermodynamic parameters describing the nanoparticle - protein interaction is a key issue for the bio-reactivity of nanomaterials having a great impact in nanosafety research.



### Biography

Speranta Tanasescu is Head of the Laboratory of Chemical Thermodynamics in the Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, Bucharest. She received his Ph.D. in Physical Chemistry – Romanian Academy in 1979; the thematic research area is oriented on activities with impact in the following domains: materials science, nanoscience and nanotechnologies, new sources of energies, nanosafety, nanomedicine etc. The obtained results by her group are significant for both the understanding of processing-structure relationships, as well as for finding key parameters in relation to bio-reactivity of the nanomaterials with impact in nanosafety research.

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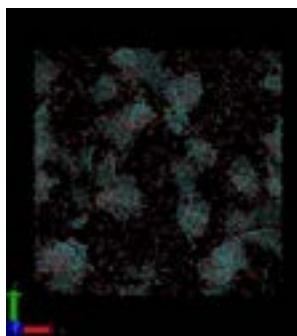
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## Formation of carbon-based nanostructures from carbon suboxide decomposition at high pressure and temperature – A ReaxFF study

Xavier Bidault and Nicolas Pineau  
CEA DAM/DIF, France

In high-pressure and -temperature conditions of detonation, carbon-rich explosives produce carbon-based nanostructures like Nano diamonds. The formation process from these organic compounds is still not clear and the published Molecular Dynamics studies are either limited to carbon condensation with no chemistry, which is quite basic, or by computer resources when modeling systems with full “carbon-hydrogen-oxygen-nitrogen” chemistry, preventing long-time simulations. As the formed nanostructures are mainly composed of carbon and oxygen (with low amounts of hydrogen and nitrogen), An intermediate system between non-reactive and full-chemistry ones can be represented by carbon sub oxide ( $C_3O_2$ ), in mixture with Argon. When modeled with a reactive force field (ReaxFF-Ig, this system catches experimental results of low-pressure detonation (~10 bar) and allows extrapolations in the high-pressure domain of solid-state high-explosive detonations (up to 60 GPa). In these extreme conditions, it appears that the formation process of carbon-based nanostructures is deeply modified and the results obtained from this reactive carbon-oxygen system give new insights on the formation of Nano diamonds.



### Biography

Xavier Bidault has his expertise in modeling and analysis of nanostructured materials by Molecular Dynamics. In order to study nanostructured optical fibers, the simple adaptive model that he developed during his Physics PhD allowed the simulations to reproduce for the first time the separation of phases of complex compositions in silica-based glasses, as experimentally observed. He now enlarges his skills to organic materials to understand how the granularity (surface energy and porosity) of a nanostructured energetic material impacts its reactivity under shock, with a focus on Nano diamond formation.

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### Notes:

11<sup>th</sup> International Conference on

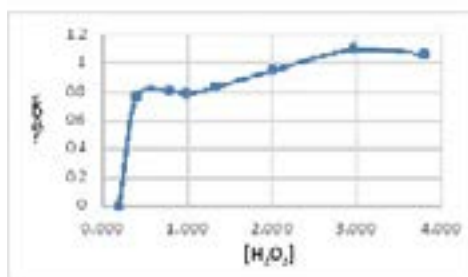
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Starch capped silver nanoparticles as colorimetric sensor for hydrogen peroxide recognition in aqueous medium

Abdelaziz Elgamouz and Baraa Hafez  
University of Sharjah, UAE

In the present study, starch capped silver nanoparticles (AgNP) were synthesized successfully and characterized by using Fourier transform infrared spectroscopy, scanning electron microscopy, dynamic light scattering and energy-dispersive X-ray Spectroscopy. The nanoparticles were used for the sensing of hydrogen peroxide based on a colorimetric technique. The nanoparticles were synthesized in a One pot reactor using  $\text{AgNO}_3$  as Ag source and sodium borohydride ( $\text{NaBH}_4$ ), as reducing agent. The silver catalytic ability for the decomposition of hydrogen peroxide was assessed using different concentration of AgNP, pH effect, temperature effect and different loads of hydrogen peroxide. The yellow-greenish color of the silver nanoparticles solution was found to change gradually to a transparent solution.



### Biography

Abdelaziz Elgamouz is an assistant Professor of bioanalytical Chemistry in the University of Sharjah. His research interest lies in coordination chemistry of macrocyclic ligands that has been a fascinating area of current research interest all over the world. The continued interest and quest in designing new macrocyclic ligands stem mainly from their use as models for protein-metal binding sites in a substantial array of metalloproteins in biological systems, as synthetic ionophores, as models to study the magnetic exchange phenomena, as therapeutic reagents in chelate therapy for the treatment of metal intoxication, as cyclic antibiotics that owe their antibiotic actions to specific metal complexation, to study the guest-host interactions, and in catalysis. Recognition of the importance of complexes containing macrocyclic ligands has led to a considerable effort being invested in developing reliable inexpensive synthetic routes for these compounds.

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### Notes:

# Sessions:

Day 1 September 07, 2017

## Advanced Biomaterials, Bio devices & Tissue Engineering | Advanced Ceramics and Composite Materials

### Session Chair

**Garcia Garcia Francisco**

University of Edinburgh, Scotland

### Session Introduction

**Title: Design of nanostructured powders and mechanical properties of WC-AISI 304 stainless steel composites**

**Ana senos**, University of Aveiro, Portugal

**Title: Thermal characterization of a thermoplastic resin for resin transfer molding in process conditions. Demonstrating of the feasibility of the technology**

**Bailleul Jean-Luc**, Laboratoire de Thermocinétique de Nantes, France

**Title: Thermoelectric oxides processed by a laser floating zone technique**

**Nuno M. Ferreira**, University of Aveiro, Portugal

**Title: LIPSS stimulate stem mesenchymal cells differentiation to osteoblasts in titanium and tantalum**

**Alberto Jorge Mora**, Universidad de Santiago de Compostela, Spain

**Title: Biological cell inspired reactors for an increasing population world**

**Garcia Garcia Francisco**, University of Edinburgh, Scotland

**Title: Synthesis of nano  $\text{CaCO}_3$  and hydroxyapatite by sol-gel methods, on spores and in 3d-printed  $\text{Ca}^{2+}$ -crosslinked pva hydrogels and their use in bone regeneration**

**Paul Sermon**, Brunel University, United Kingdom



11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

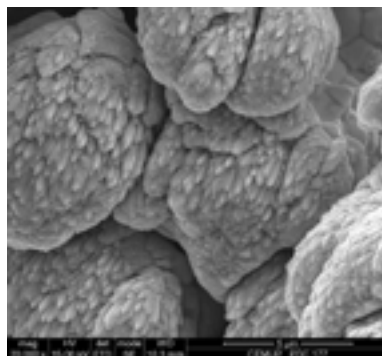
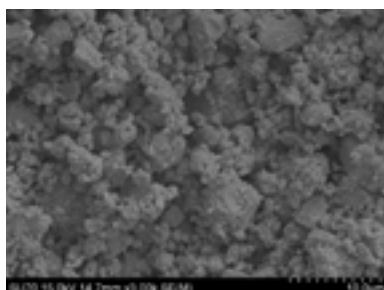
September 07-08, 2017 | Edinburgh, Scotland

## Design of nanostructured powders and mechanical properties of WC-AISI 304 stainless steel composites

Ana M.R. Senos

University of Aveiro, Portugal

Cemented carbides are constituted by WC and a metallic binder usually processed through powder metallurgy routes. The good compromise between hardness and toughness achieved in cemented carbides designates the common use to cutting, machining and wear applications. The increasing application demands require not only materials with improved properties but also efficient processing techniques. The improvement of mechanical properties, namely hardness, can be achieved through grain size reduction up to the nanoscale range. In the present work nanostructured powders of WC and stainless steel (SS) have been prepared using two routes: high energy ball milling (HEBM) to produce nanometric particles of WC and SS; and an innovative sputtering coating technique (SC) to coat micrometric WC particles with nanometric SS. For comparison, powders in the micro/submicrometer range were also prepared by conventional milling (CM). Composites of these powders were shaped by pressing and thermal consolidated using vacuum sintering. The final phase composition and microstructure were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM/EDS), respectively, together with X-ray mapping for elemental distribution and electron backscatter diffraction (EBSD) for the grain size distribution. High resolution transmission electron microscopy (HRTEM) was also used for grain boundaries inspection and access the nanometric details of the microstructure. Composites from the different powders (HEBM, SC and CM) showed very different values of hardness, HV30, and toughness, KIC, varying from extremely hard parts for the HEBM composites, to impressive high tough composites for the SC parts. These mechanical responses are discussed taking into account the structure/microstructure and grain boundaries details leaded by the designed powder morphology.



SEM micrographs (a) WC-12SS mixture prepared by HEBM; (b) WC powder sputter-coated with 12SS.

### Biography

Ana Senos is Associate Professor at the Dep. Materials and Ceramic Engineering, University of Aveiro, Portugal. She has been involved in the investigation of ceramics and nanocomposites processing, on the topics of sintering kinetics, microstructural development, grain boundary design, constrained sintering, and the relation with the electrical answer and mechanical behavior of materials. Current interests are focused on development of nanostructured materials for structural, electrical and nuclear applications and on the study of grain boundary phenomena in electronic functional materials (2D, 3D), for microwave and energy applications. Is author (co-authored) of more than 130 publications, including 3 Book Chapters, 103 papers (92 from SCI), 19 proceedings and 2 patents, with ca. 1400 citations (h-index=22). She has about 130 communications as oral and poster presentations or as invited speaker.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Thermal characterization of a thermoplastic resin for resin transfer molding in process conditions. Demonstrating of the feasibility of the technology

Jean-Luc Bailleul<sup>1</sup>, Jalal Faraj<sup>2</sup> and Nicolas Boyard<sup>3</sup><sup>1,3</sup>LTEN, Nantes, France<sup>2</sup>ETG, Beirut, Lebanon

Composites materials pieces based on thermoplastics resins are suitable candidates to replace iron parts in the automotive sector for the purpose of reducing weight and hence to reduce CO<sub>2</sub> emissions. But, the use of such composite material used in the automotive sector is notably determined by the total cost of the pieces. So, new materials such as low viscosity thermoplastics or reactive thermoplastics resins are developed to give an answer. These materials needs also the development of adapted processing methods like resin transfer molding (RTM) and compacting resin transfer molding (C-RTM). In this presentation we deal with the thermal characterization of low viscosity resin, and more specially its crystallization kinetics, in wide temperature range with an Avrami model. The study of its density evolution during crystallization, according to the pressure and the temperature, is also presented. Then we present new devices developed to prove the feasibility of thermoplastics resins processing by RTM. The experimental thermal measurements during an injection demonstrate the accuracy of our thermal model and of its thermal parameters.

### Biography

Jean-Luc Bailleul is working on composite material processing since twenty year. Specially on the mastering of thermal cycle to control final pieces qualities in terms of their final mechanical properties and in terms of cycle time. Thus, he has developed a phenomenological model to describe heat generation during thermosets resins transformation. The specificity of his laboratory is the development of experimental tests benches to understand the physical phenomena that occurs in composite materials during their transformation. Since ten years he develops also some works on composites materials recycling. The result of all his works is that he has now a good hindsight on thermal phenomena influence on polymer processing.

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### Notes:

11<sup>th</sup> International Conference on

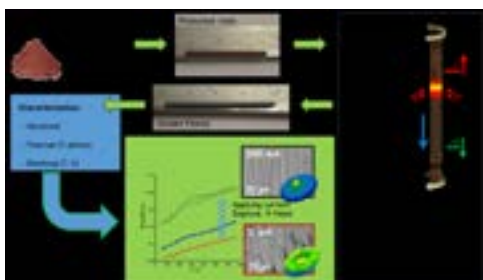
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Thermoelectric oxides processed by a laser floating zone technique

N.M. Ferreira<sup>1</sup>, S. Rasekh<sup>2</sup>, A.V Kovalevsky<sup>3</sup>, F.M. Costa<sup>4</sup>, M.A. Madre<sup>5</sup>, J.C. Diez<sup>6</sup> and A. Sotelo<sup>7</sup><sup>1,2,3,4</sup>Universidade de Aveiro, Portugal<sup>5,6,7</sup>CSIC-Universidad de Zaragoza, Spain

Oxide ceramics are very promising materials for new thermoelectric devices, as they exhibit high Seebeck coefficient and could present relatively low electrical resistivity, as well as high chemical stability at high temperatures. They show anisotropic thermoelectric properties linked to their layered structures. Therefore, texturing methods developing oriented grains, such as grain growth processes have already shown their applicability to this kind and similar compounds. Among these methods, the laser floating zone (LFZ) melting technique has been found to be very promising to tune up the performances of these compounds, especially in the Co-oxide based materials studied in the last years in our laboratories. In this work, some examples highlighting the versatility and usefulness of LFZ technique and the improvements on the thermoelectric performances of textured materials will be shown. This technique allows obtaining very dense, and well textured thermoelectric composite materials. In spite of the well-known incongruent solidification of this family of materials, the as-grown samples possess high thermoelectric properties which can be further enhanced by an adequate annealing procedure, leading to nearly single phase materials. These microstructural modifications produce an important improvement of power factor when compared with materials prepared through conventional techniques. Moreover, this processing technique also shows good prospects to be applied in modules construction.



### Biography

Nuno Ferreira a PhD (2014) in Physics Engineering, nowadays, a pos-doc researcher at I3N, Physics Department and CICECO – Materials science and Ceramics Department at Aveiro University – Portugal. Had participated as collaborator and fellowship in several R&D projects on material science. Experience on study and development of ceramic based materials prepared through conventional methods (melting, solid stated) and focus in laser processing (crystal growth – LFZ and surface sintering). Present sample characterization skills on different techniques such as, electrical conductivity and magnetic properties of various oxide materials. Current focus materials: thermoelectrics, ferroelectrics and glass matrices doped with transition metals and rare earth for energy storage and conversion applications. Main expertise is related to magnetic and electrical properties of materials and laser processing.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## LIPSS stimulate stem mesenchymal cells differentiation to osteoblasts in titanium and tantalum

Alberto Jorge-Mora<sup>1</sup>, Jesús Pino-Mínguez<sup>2</sup>, Rodolfo Gomez-Vaamonde<sup>3</sup> and Daniel Nieto<sup>4</sup>

<sup>1,2</sup>Universidad de Santiago de Compostela

<sup>3</sup>Santiago University Clinical Hospital, Spain

<sup>4</sup>Universidad de Santiago de Compostela, Campus Vida, Spain

Orthopaedic surgery has grown from the hand of new materials that made possible to perform procedures as total hip replacement with feasibility. These procedures are common in most orthopaedic departments, and more than 70 000 hip or knee replacements are performed in Spain every year. The survival of these implants is critical to prevent loosening and the need for revision arthroplasty. The ideal surface to interact with bone has not been created. We created laser induced periodic surface structures (LIPSS) in the surface of titanium and tantalum to study the behaviour of stem cells compared to polished surfaces. We created 12 discs of each material and polished them. Later we created LIPSS in 6 discs of each material. We cultured them in human stem cells in a concentration of 25000 cell per cm<sup>2</sup> for 20 days. We determined MTT, TNF- $\alpha$ , alkaline phosphatase, IL-6, osteopontin and osteocalcin every 5 days until the day 20. We confirmed outcomes behave as a normal distribution after applying the Kolmogorov Smirnov test. We compared materials and surfaces with the T-student test. We accepted a difference of 0.05 as significant. LIPSS created increase statistically cell metabolism (best values in MTT assay) and decrease inflammatory response to the material (IL-6 and TNF- $\alpha$  values). Collagen is produced in more quantity and cells differentiate to osteoblast easily. These differences are seen from the beginning until the endpoint (day 20). When LIPSS improved osteogenic properties of titanium and tantalum compared to smooth surfaces.

Parameter	Day 0	Day 5	Day 10	Day 15	Day 20	Day 0	Day 5	Day 10	Day 15	Day 20
MTT	0.4897	0.3420	0.5884	0.4090	0.6455	0.2413	0.7595	0.5464	0.3945	0.5464
IL-6	0.0106	0.0116	0.0200	0.0218	0.0340	0.0436	0.0280	0.0390	0.0340	0.0340
TNF-ALFA	0.0164	0.0211	0.0100	0.0118	0.0290	0.0196	0.0230	0.0230	0.0230	0.0230
PCN	0.0000	0.0000	0.2066	0.1830	0.2067	0.1288	0.1426	0.1019	0.1019	0.1019
OC	0.0448	0.0448	0.7827	0.5891	0.7183	0.5152	0.8525	0.6954	0.6954	0.6954
OC	0.3079	0.2032	0.2317	0.1865	0.5240	0.2362	0.8031	0.6268	0.6268	0.6268
OSP	0.4177	0.3114	0.3940	0.2130	0.5448	0.4049	0.2340	0.6311	0.6311	0.6311

### Biography

Alberto Jorge is an orthopaedic Surgeon with special interest in biomaterials. He is focusing every effort in the study of the behaviour of surface modifications in the field of orthopaedic surgery. Previously he performed different modifications in PMMA to create composites with hydroxyapatite to prevent fibroblastic response (Pino et al 2015). Nowadays he is dedicated to laser modification of metals and cermets to increase anisotropic osteointegration of implants.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

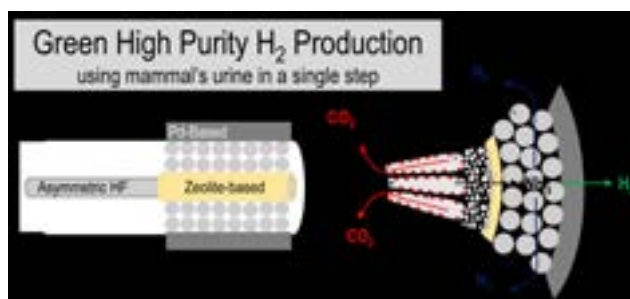
September 07-08, 2017 | Edinburgh, Scotland

## Biological cell inspired reactors for an increasing population world

**F.R. García-García**

The Edinburgh University, UK

Dr Francisco R. García-García research seeks sustainable solutions to today's emission control and energy production challenges by mimicking biological cell strategies. Biological cells can be seen as enhanced multifunctional reactors specifically designed to solve fundamental chemical engineering issues such as thermodynamic limitations, catalyst deactivation, and product separation. For example, cells can overcome the thermodynamic limitations because the reaction sites are enclosed within the cell membrane, which is permeable to some of the reaction products. Likewise, cyclic vs linear pathways allow a quick and economic solution to chemical problems. While these approaches are common in cells, they are only sporadically applied technologically in a purposeful manner. The aim of Dr Francisco R. García-García research group is to design, develop and fabricate multifunctional catalytic reactors inspired by how biological cells work, which allows the integration of multi-processes in a single device. The integration of multi-process (reaction, regeneration and separation) in a single reactor enables the intensification of the overall process, making it safer, cleaner, smaller and cheaper. So far the difficulty of combining chemistry, materials science and engineering knowledge in a single unit has prevented the full development of this concept. In this respect, Dr Francisco R. García-García is recognized for his knowledge in the area of gas phase heterogeneous catalysis, new materials development, membrane technology and chemical looping in the interphase between chemistry and chemical engineering. The below biological cell inspired multifunctional reactor enables the production of high purity hydrogen by using mammal's urine as a feedstock. The integration of multi-process (i.e. reaction and separation) in a single unit allows hydrogen production to be done in a single step.



### Biography

Dr Francisco R. García-García is a Lecturer in Chemical Reaction Engineering at the School of Engineering at University of Edinburgh. He holds an MSc in Chemistry by the Autónoma University of Madrid and a PhD in Chemical Engineering by the Institute of Catalysis and Petroleum-chemistry, CSIC. He gained his first post-doctoral experience working at the Department of Chemical Engineering of Imperial College London. In this period, he focused in the design and development of catalytic multifunctional reactors for hydrogen production. Afterwards, he worked as a Senior Scientist at Johnson Matthey in the Emissions Control Department. Despite having a very rewarding experience working in industry, he soon realized that he preferred to be involved in more fundamental science and he moved back to the academia. Hence, he joined the UK Catalysis Hub as a research fellow working at the Chemical Engineering Department at Cambridge University, and at the Chemical Engineering Department at Newcastle University. During this time his research focused in chemical looping reforming for syngas and hydrogen production.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Synthesis of nano CaCO<sub>3</sub> and hydroxyapatite by sol-gel methods, on spores and in 3D-printed Ca<sup>2+</sup>-crosslinked PVA hydrogels and their use in bone regeneration

P.A.Sermon, I.AL-Timimi, U.Onwukwe, C.Sheng and L.Mukendi  
Brunel University, UK

Some have used sol-gel synthesis to give injectable hydroxyapatite (HAp) nanoparticles (NPs) using aqueous solutions of Ca(CH<sub>3</sub>COO)<sub>2</sub>·2H<sub>2</sub>O to which was added 1,2-ethandiol, chelator ethylenediaminetetraacetic acid (EDTA), triethanolamine and then Na<sub>2</sub>HPO<sub>4</sub> that could be spin- or dip-coated on various substrates. Others suggest that inorganic-organic combinations are better for initiating bone replacement treatments. Some have chosen HAp deposited on bacterial-cellulose, but that required cellulose treatment with citrate ions to increase Ca<sup>2+</sup> take-up and even then the product had a low (1.2) Ca:P ratio. Here we compare HAp that is 1. sol-gel-derived nanoparticles (NPs). 2. generated on the surface of organic harvested Portobello mushroom spores (PMS); after PMS washing in water and then acetone, they were infiltrated with 5 mL (55mM) CaCl<sub>2</sub> solution for 1h with stirring at 310K to give Ca<sup>2+</sup>/PMS, filtered, dried, and then infiltrated with a 55mM Na<sub>2</sub>CO<sub>3</sub> to give CaCO<sub>3</sub>/PMS and finally with a 13mM Na<sub>2</sub>HPO<sub>4</sub> to give HAp/PMS with Ca:P=1.7. 3. ultrasonically removed from the surface of the HAp/PMS and is then dip- or spin-coated onto a range of substrates. 4. produced in 3D printed PVA hydrogels that are pre-crosslinked by Ca<sup>2+</sup> [4,5] and then converted to HAp/PVA by alternate infiltration with aqueous solutions (120mM) of Na<sub>2</sub>HPO<sub>4</sub> and CaCl<sub>2</sub> at pH=7.4 and 310K [6]. Product HAp was characterized by FTIR (where peaks at 873cm<sup>-1</sup> (vibration stretching mode of P-O) and 559 and 433 cm<sup>-1</sup> (vibration bending mode of O-P-O in the PO<sub>3</sub><sup>-3</sup> were seen), Raman, TEM, SEM-EDX (Ca:P), XRD and TGA-DSC and biocompatibility with body fluids and enhancement of bone growth with improved mechanical properties. The wider opportunities for nanomaterials synthesis using bio templates and 3D printed PVA hydrogels are considered.

### Biography

Professor Paul A. Sermon was born in Caversham in 1945. He was educated at Westminster City School, Bangor University and University of Bristol (PhD, DSc). He was Professor of Physical Chemistry at the University of Surrey, where his research concentrated on bottom-up nanotechnological routes to catalysts, sensors and biofuels, until the autumn of 2010. He then became Professor of Nanomaterials at the Wolfson Materials Processing Centre in 2011. His research is now focused in nanomaterials and biomimetic nanomaterials with useful forensic, catalytic and photocatalytic properties. This research is supported by Government Agencies and the Royal Society. On Thursday 10th November 2011 at a dinner at the Royal Society, it was announced that he was a recipient of a Royal Society Brian Mercer Feasibility Award.

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### Notes:

# Sessions:

Day 1 September 07, 2017

## Materials Processing and characterization | Materials for Energy application & Energy storage

Session Chair  
**Alexandre Maitre**  
University of Limoges, France

### Session Introduction

**Title: Atomic layer deposition routes to monolithic integration of crystalline oxides on semiconductors**

**John Ekerdt**, University of Texas at Austin, USA

**Title: Tailoring compatibility in ultrapermeable polymer blends to switch off plasticization and physical ageing**

**Lau Sam**, University of Edinburgh, Scotland

**Title: Mechanism of spark plasma sintering of high temperature ceramics such as carbides**

**Alexandre Maitre**, University of Limoges, France

**Title: Testing methodologies for thermo-mechanical fatigue evaluation in advanced aerospace materials**

**Mark Whittaker**, Swansea University, United Kingdom

**Title: Characterization of energy materials by neutron scattering**

**Martin Jones Owen**, Science and technology facilities council, United Kingdom

**Title: Permanent magnets in energy applications for the clean environment**

**Spomenka Kobe**, Jožef Stefan Institute, Slovenia

11<sup>th</sup> International Conference on

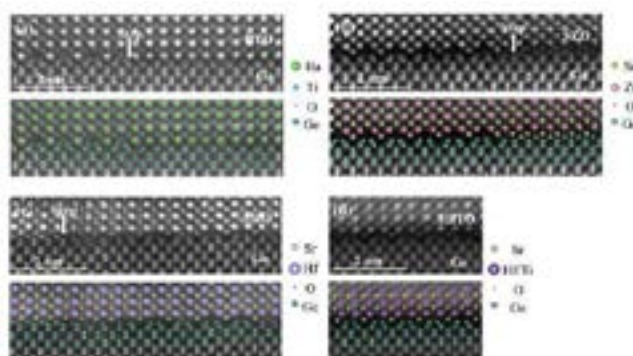
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Atomic layer deposition routes to monolithic integration of crystalline oxides on semiconductors

John G. Ekerdt, Shen Hu, Edward L. Lin, Pei-Yu Chen, Agham Posadas and Alexander A. Demkov  
University of Texas at Austin, USA

The semiconductor industry faces new challenges in the sub-10 nm era as scaling will no longer dominate performance improvement. New materials provide opportunity to improve performance with minimal architectural overhaul. For example, high-mobility channels of Ge and III-V semiconductors can provide both lower power consumption and faster computing speeds. In certain applications significant advantages are gained by monolithic integration of the oxides directly on the substrates that will host other devices/components. Perovskite oxides offer a wide range of properties from high-k to multiferroic affording the device designer a suite of possibilities, and are particularly important due to their common structure and lattice-matching with common semiconductors. The gallium nitride device applications will require a dielectric to passivate the nitride surface. Atomic layer deposition (ALD) allows for growth of perovskite oxides and rare earth oxides in a chemical deposition process that is scalable and manufacturable. It is possible to grow crystalline perovskites directly on Ge(001) by ALD. Using this approach we have been able to deposit STO, BaTiO<sub>3</sub>, SrHfO<sub>3</sub>, Sr(HfTi)O<sub>3</sub>, and SrZrO<sub>3</sub> directly on Ge(001). We will discuss the growth and properties of the perovskite layers directly on Ge(001), and will discuss the interface chemistry and structure that likely controls the interfacial reactions that allow for crystalline film formation. It is also possible to grow crystalline rare earth oxides directly on GaN(0001) by ALD. We report approaches to growing crystalline, hexagonal and cubic Er<sub>2</sub>O<sub>3</sub> on wurtzitic gallium nitride, GaN (0001). As with growth of perovskites on Si and Ge, atomically-thin intermetallic compounds comprised of Group 1 or 2 elements and Group 13-15 elements to facilitate wetting and direct the crystalline growth, in this case the [111] growth direction of the oxides on GaN (0001). This talk will describe the growth, structures and properties of crystalline oxides grown by ALD.



HAADF STEM images showing the interface of BaTiO<sub>3</sub> (BTO) (a), SrZrO<sub>3</sub> (SZO) (b), SrHfO<sub>3</sub> (SHO) (c) and SrHf<sub>0.55</sub>Ti<sub>0.45</sub>O<sub>3</sub> (SHTO) (d) films grown by ALD on Ge (001) substrates. White arrows mark the position of a single layer Ge surface step. Structural models below each image illustrate the interface structure in particular showing the change in periodicity of the Ge (001) substrate surface and the location of the Ba (or Sr) atomic columns between the Ge dimers. S. Hu et al., J. Chem. Phys. 146, 052817 (2017).

### Biography

John G. Ekerdt is Associate Dean for Research in Engineering and the Dick Rothwell Endowed Chair in Chemical Engineering at the University of Texas at Austin. He has more than 300 refereed publications, two books and three book chapters, and seven U.S. patents. He has supervised 48 Ph.D. and 8 M.S. students. Current research interests focus on the surface, growth and materials chemistry of metal, dielectric and perovskite films and nanostructures. The work seeks to: 1) develop and understand the reactions and chemistry that control nucleation and growth of films and nanostructures, and 2) understand the properties of these materials and relate the properties to structure, bonding and growth.

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### Notes:



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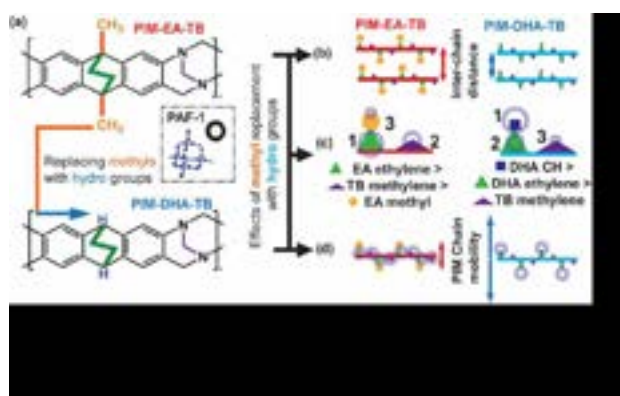
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Tailoring compatibility in ultrapermeable polymer blends to switch off plasticization and physical ageing

Cher Hon Lau<sup>1</sup>, Mariolino Carta<sup>1</sup>, Richard-Malpass Evans<sup>1</sup>, Elsa Lasseugeuette, Maria-Chiara Ferrari<sup>1</sup>, Neil B<sup>1</sup>, Kristina Konstas<sup>2</sup>, Cara M. Doherty<sup>2</sup> and Matthew R. Hill McKeown<sup>2</sup><sup>1</sup>University of Edinburgh, Scotland<sup>2</sup>CSIRO, Australia

Despite the rapid evolution of material science, it remains difficult to deploy new polymers that are inadequate to meet the stringent demands of industrial membrane separations. Polymer membranes must be ultrapermeable, selective, and resistant to both physical aging, and plasticization. Polymers with intrinsic microporosity (PIMs) are ultrapermeable, yet vulnerable to physical aging and plasticization. Here we show that aging and plasticization in PIMs can be switched on and off through compatibility with a microporous polymer, porous aromatic frameworks (PAFs). By replacing bulky methyl groups with smaller hydro groups, we remove the ability of a PIM polymer matrix to interact with PAFs; accelerating both physical aging and plasticization. Meanwhile PAFs tailors physical aging and annihilates plasticization in the original methylated PIM via physical interactions at specific locations on the PIM polymer chains. This benefits hydrogen recovery at realistic operating conditions; enabling the implementation of polymer membranes as a stand-alone separation technology, a paradigm shift from existing hybrid methods.



### Biography

Dr. Cher Hon (Sam) Lau is a Chancellor's Fellow at the University of Edinburgh. His current research focuses on the scale-up production of microporous materials that are compatible with various polymer matrices, and polymer membranes for liquid separations. Prior his appointment at UoE, he spent 5 years at the Commonwealth Scientific Industrial Research Organisation (CSIRO), Australia as a post-doctoral fellow, subsequently as a research scientist. At CSIRO, he discovered the world's first anti-aging membranes for gas separations and solvent purifications. His anti-aging membrane research is also the cornerstone of membrane research and commercialization efforts in CSIRO. He also co-led several industrial projects working on gas separation and capture using porous frameworks, scale-up production of porous nanoparticles, and membrane separations. He received his Ph. D. degree from the Chemical Engineering department at the National University of Singapore in 2012. He has published more than 20 papers and 4 patents on membrane science and technology in high impact journals.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Mechanism of spark plasma sintering of high temperature ceramics such as carbides (ZrC, B4C)

Alexandre Maitre, Nicolas Pradeilles and Guy Antou  
University of Limoges, France

Spark Plasma Sintering (SPS) has proved its efficiency on the sintering of various materials which were known to be difficult to sinter without additives. In this presentation, the investigation of some thermomechanical properties will be illustrated on two different carbides: Zirconium carbide and boron carbide. Zirconium Carbide is interesting for high temperature application. Zirconium carbide ( $ZrC_x$ ) and oxycarbide ( $ZrC_xO_y$ ) carbide was synthesized by carbo-reduction of zirconia and carbon and was then sintered by SPS. A complete study including composition, particles size evolution was done. The kinetics of spark plasma sintered ceramics has been investigated. A change of densification mechanism appears during the intermediate and final sintering stages. During this last stage, the deformation mechanism is similar to the one involved during creep of dense ceramics. The comparison of densification and creep strain rates seems to show that no specific effects strongly enhance strain rate during the final densification stage of Spark Plasma Sintering. Boron carbide is a promising material for moderator in nuclear industry. The influence of preparation before SPS was studied: a liquid way was studied and compared. Different solvents were tested and green bodies were obtained. During this sintering, different chemical reactions were observed: oxides present in the native powder react and the composition of the carbide evolves. In a second step, thermomechanical properties were determined.

### Biography

Alexandre Maître is professor at the Science of Ceramic Processes and Surface Treatments laboratory at Limoges in France. His thesis diploma (1995-1998) was devoted to the kinetic and thermodynamic aspects of the synthesis of transition metal carbides by carbothermal reduction. In October 2000, he obtained a permanent position as CNRS researcher at the Laboratory of Chemistry of Inorganic Solids at Nancy to develop investigations concerning the thermodynamic modelling, the electrochemical behaviour in corrosive environment, the metallurgical aspects of lead-based alloys. In September 2004, he became assistant professor in SPCTS to implement research activities about the elaboration by Polymer Derived Ceramics (PDCs) route and the mechanisms of sintering of high temperature ceramics. His scientific production (h index: 16) is now composed of 92 publications in international journals, 22 invited conferences, 65 oral communications, 3 chapters of books, 3 grants, etc. He was responsible for at least 15 national or international projects.

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### Notes:

11<sup>th</sup> International Conference on

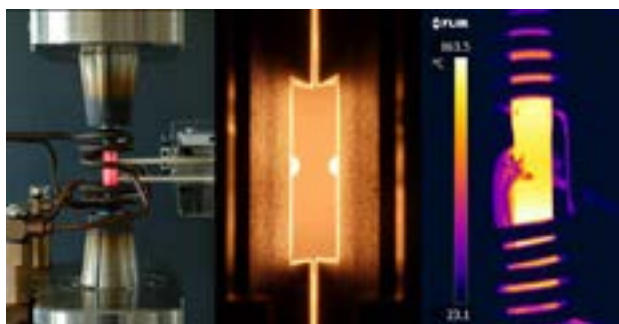
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Testing methodologies for thermo-mechanical fatigue evaluation in advanced aerospace materials

Mark Whittaker, Jonathan Jones, Ashley Dyer and Jennie Palmer  
Swansea University, UK

Fatigue failures are common within structural components used throughout a range of industrial sectors, and are often a critical design criterion during the specification and development stage of a new product. However, most mechanical testing is performed under isothermal conditions which may not be truly representative of in service conditions. Thermo-mechanical fatigue (TMF) testing offers the opportunity for the evaluation of a range of advanced material under more appropriate thermal cycles, hence providing more appropriate lifing approaches to ensure component integrity. TMF tests however, are complicated and difficult to perform, with much consideration necessary to understand the complex interactions of issues such as the heating/cooling method, the phase angle between thermal and mechanical strains/stresses, temperature measurement techniques and cycle frequencies. Over the past 15 years, the Institute of Structural Materials at Swansea University has devoted significant effort in a number of developmental programmes which have led to internationally recognised expertise in experimental setup and lifing approaches. Consideration in this paper is given to the experimental difficulties associated with using traditional techniques for temperature and crack length measurements (thermocouples and direct current potential difference techniques) and the possibility of utilising more innovative approaches such as thermography is discussed. Research has shown that it is difficult to design a single solution for TMF testing due to the numerous testing requirements that include peak cycle temperature, heating/cooling rate, and the impact of electromagnetic fields associated with induction coils. As such, TMF experiments are often by their very nature, bespoke. Future developments such as the generation of a validated code of practice for crack growth measurements under TMF loading are also discussed.



### Biography

Dr Whittaker joined Swansea University in 2003 and has produced over 60 publications including an invited book chapter and 40 papers in leading international journals on topics including High Temperature Lifing, Thermo-Mechanical Fatigue and Modern Creep Lifing Approaches. He is also a Board Member of the IOM3 Structure and Properties of Materials Committee. Current research programmes involve sponsorship from EU Clean Skies, Rolls-Royce, EPSRC and ATI. Dr Whittaker has over 15 years of experience in a wide range of alloys and is leading the development of a code of practice for thermo-mechanical fatigue crack propagation testing. He is also heavily involved in creep lifing of alloys for the power generation/aerospace sectors, with particular expertise in property extrapolation using the recently developed 'Wilshire equations'.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Characterization of energy materials by neutron scattering

**Martin Owen Jones**

Science and Technology Facilities Council, UK

The ISIS neutron and muon facility is ISIS is a world-leading centre for research in the physical and life sciences at the STFC Rutherford Appleton Laboratory. Its two target stations give an unrivalled breadth of neutron science capabilities and have provided the blueprint for future neutron scattering facilities worldwide. ISIS supports a national and international community of more than 3000 scientists for research into subjects ranging from clean energy and the environment, pharmaceuticals and health care, through to nanotechnology and materials engineering, catalysis and polymers, and on to the fundamental studies of materials. The extensive characterisation facilities include neutron and muon instruments that can determine structure, molecular motion and ionic mobility at extremes of temperature and pressure. Neutron tomography experiments can also be performed to image devices to a resolution of 40 microns.

This presentation will introduce the ISIS neutron and muon facility at the Rutherford Appleton Laboratory, including descriptions of the instruments, techniques and capabilities at the facility. The characterisation of energy materials will be explained through a number of case studies ranging from solid oxide fuel cells, through electrolyte materials to conventional and unconventional hydrogen storage materials.

### Biography

Martin Owen Jones is a professor at Science and Technology Facilities Council, UK. His international experience includes various programs, contributions and participation in different countries for diverse fields of study. His research interests as a Scientist reflect in his wide range of publications in various national and international journals.

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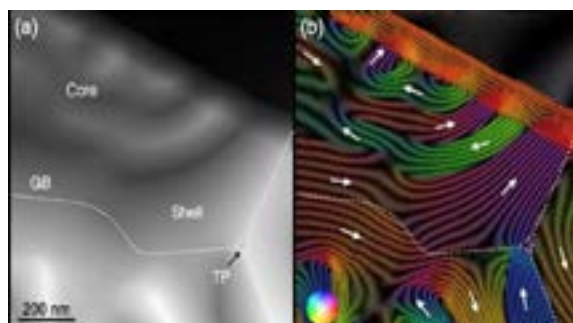
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Permanent magnets in energy applications for the clean environment

Spomenka Kobe, Marko Soderžnik and Kristina Žagar  
Jožef Stefan Institute, Slovenia

Rare-Earth Transition Metals permanent magnets are vital components in the rapidly-developing renewable energy sector, where the motors for electric vehicles and the generators in wind turbines require strong magnets with the ability to operate at temperatures well over 100°C. To achieve high coercivity, remanence and consequently high-energy product at elevated temperatures the addition of heavy rare earth (HRE) to the basic Nd-Fe-B composition is needed. On the list of Critical Raw Materials published by the EC in 2014, HRE is on the very top of it. To drastically reduce the use of HRE we focused on developing a new method, which should enable us to achieve the properties needed for high-temperature application with the lowest amount of scarce elements. The significant progress was attained by using electrophoretic deposition as a method for accurately positioning the HRE on the surface of a sintered Nd-Fe-B magnet before its diffusion into the microstructure. After the additional annealing, this process locally increased the coercivity of final magnet, thereby substantially reducing the dependence on the HREs, Dy, and Tb<sup>1-3</sup>. By our new inventive technique further transferred to a pilot production, we could minimize the amount of HRE used, down to 0.2 at %, the improvement of coercivity was 30 % with minimal loss in remanence. The total saving of the HRE is 16-times less need for the same performance, which is a significant contribution to the world economy and clean environment. In studying the mechanism for such an improvement in coercivity without significantly decreasing the remanence, a detailed microstructure investigation was performed by using high-resolution transmission microscopy and analysis at the nano level (Fig. 1). Besides the use of these new developed high energy magnets for electric and hybrid cars and the wind turbine generators the important application is also as the source of the magnetic field in the development of the new magnetic cooling devices.



**Fig.1:** Electron Holography of the core/shell region. (a) Total phase image with marked location of the grain boundaries (GB) and the triple pocket (TP). (b) Reconstructed phase showing the magnetic flux distribution and color maps. The contour spacing is  $\pi/2$ .

### Biography

Prof. Spomenka Kobe is Scientific Advisor, Head of the Department for Nanostructured Materials and a Member of the Scientific Council at the Jožef Stefan Institute. She is a full professor at the International Postgraduate School "Jožef Stefan". Prof. Kobe is the Leader of the National Research Programme "Nanostructured Materials". She is the recipient of two State Awards for Scientific Research and two Innovation Awards from industry for the successful transfer of technology. Her scientific work is documented in more than 150 refereed publications, 7 chapters in a book and invited talks at international conferences. Her applied research achievements include 5 patents (2 EP), 3 innovations and 5 successful transfers of technology to the industrial production. Prof. Kobe is also the previous President of the Academic Society for Science and Engineering (SATENA) and an acting Vice-Chair for the European Commission. She supervised 15 doctoral students.

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### Notes:

## Advanced Materials Engineering | Materials Science and Engineering | Emerging Areas of Materials Science

Session Chair  
**Masumi Saka**  
Tohoku University, Japan

Session Chair  
**Klaudio Bari**  
University of Derby, UK

### Session Introduction

**Title: Interaction of nanoparticles with amino acids and a physiologically important model protein studied by spectroscopic techniques**

**Karolína M. Šišková**, Palacký University in Olomouc, Czech Republic

**Title: Kovacs effect and the relation between glasses, supercooled liquids and crystals**

**Francesco Aliotta**, Istituto per i Processi Chimico-Fisici, Italy

**Title: Co-electrodeposition of Zn-rich Cu-Zn-Sn metallic alloy and its conversion to  $\text{Cu}_2\text{ZnSnS}_4$  and  $\text{Cu}_2\text{ZnSnSe}_4$  photovoltaic absorber films**

**Ali Rakhshani**, Kuwait University, Kuwait

**Title: Surface mechanics design of metallic materials by cavitation peening**

**Hitoshi soyama**, Tohoku University, Japan

**Title: Fatigue analysis of a failed connecting rod in race car engine**

**Klaudio Bari**, University of Derby, United kingdom

**Title: Crack / Damage evaluation and micro-materials fabrication in the relation with electric field**

**Masumi Saka**, Tohoku University, Japan

**Title: Hydrogen production from water using the sun via photocatalytic processes on Au/g- $\text{C}_3\text{N}_4/\text{TiO}_2$  materials**

**Valerie Keller**, Institute of Chemistry and Processes for Energy, Environment and Health, France

**Title: Advanced polydimethylsiloxane-urea copolymer based masterbatches with multiple functionality**

**Hans-Joachim Radusch**, MLU Halle, Germany

**Title: Sculpture art and fashion design**

**Mayssa El Fare**, Damietta University, Egypt

**Title: Material science and fashion design**

**Nashwa El Shafey**, Damietta University, Egypt

**Title: Structures, interactions and optical responses from polymer and polymer nanocomposites**

**Sarathi Kundu**, Institute of Advanced Study in Science and Technology, India

**Title: Recent advances in polylactic acid based blends, composites and nanocomposites for packaging and barrier applications**

**Kartikey Verma**, Chandigarh University, India

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

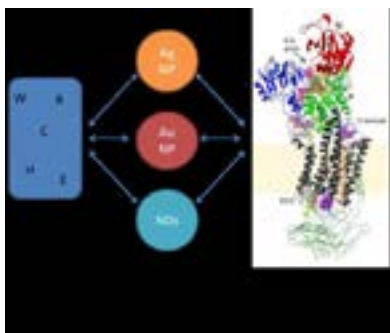
September 07-08, 2017 | Edinburgh, Scotland

## Interaction of nanoparticles with amino acids and a physiologically important model protein studied by spectroscopic techniques

**Karolína M. Šišková**

Palacký University in Olomouc, Czech Republic

Nanoparticles (NPs) are currently the topic of interest of a bundle of research papers and proposals. There are persistent rumors about NPs toxicity and ecotoxicity, concerns about their increasing release into the environment and attempts to their risk assessment. Many researchers often test the impact of different kinds of NPs on cells, tissues, organs, and/or directly on whole organisms. However, in order to understand the possible NPs impacts it is necessary, in my opinion, at first to evaluate the interaction of NPs with one type of the basic units of all organisms and their cells, i.e. amino acids. Furthermore, it is important to elucidate whether and how can NPs affect the conformation of proteins (their secondary and tertiary structure). Only after gaining such information, the assessment of NPs toxicity and ecotoxicity could be meaningful. In this study, the interaction of synthesized and commercially available nanoparticles with selected amino acids and a physiologically important transmembrane protein, the sodium/potassium pump (Na<sup>+</sup>/K<sup>+</sup>-ATPase) will be investigated by using several spectroscopic techniques. The sodium/potassium pump is an enzyme which is ubiquitous in all animal cells and its malfunctions are related to many diseases such as hypertension, diabetic neuropathies, renal failure, neurological disorders etc.



### Biography

Karolína M. Šišková has her expertise in nanoparticle synthesis, characterization, application and in vibrational spectroscopy. She published more than 40 papers as the main author or co-author in impacted scientific journals and presented more than 20 oral contributions and 8 posters on different nanomaterial and spectroscopic conferences and meetings. She graduated in physical chemistry from the Charles University in Prague and in INTER//BIO from the Université Pierre et Marie Curie, Paris VI, in 2006. In 2014, she was awarded the conferment of associate professor degree in physical chemistry. Her h-index is 15 and the number of citations 515 (without self-citations) according to the Web of Science on 20th December 2016. Coming back from her maternity leave in September 2016, she started to work at the Department of Biophysics, Faculty of Science, Palacký University in Olomouc, Czech Republic.

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11<sup>th</sup> International Conference on

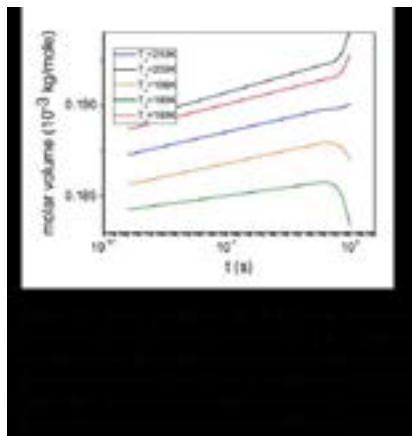
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Kovacs effect and the relation between glasses, supercooled liquids and crystals

Francesco Aliotta  
CNR-IPCF, Italy

We revisit Kovacs' effect, which concerns the way the volume of a glass-forming liquid, originally driven out of equilibrium, changes with time while the system evolves towards a metastable state. The theoretical explanation of this phenomenon has attracted a deep interest even in recent years, because of its relation with some subtle aspects of the still elusive nature of the glass transition. In fact, even if there is a rather general consensus on the fact that what is experimentally observed on cooling is the dramatic effect produced by the dynamical arrest of slower degrees of freedom over the experimental time scale, it is not at all obvious whether this phenomenology can be justified by an underlying (possibly, high order) phase transition at a lower temperature. We show how the phenomenon investigated by Kovacs can be explained in terms of the relaxation undergone by slow motions, on a time scale comparable with the experimental time windows. The results from a simple model system, namely o-therphenyl, are compared with indications from other glass formers, including water. The mechanisms underlying the formation of crystals (dendrites) when a supercooled liquid escape metastability are also explored within the adopted perspective. The ability of a simple out-of-equilibrium approach in reproducing a wide class of phenomena related with the glass transition suggests the idea that the hypothesis of a thermodynamic phase transition should be reconsidered in favor of alternative scenarios.



### Biography

Francesco Aliotta has his main expertise in the field of Thermodynamics of irreversible processes. In particular he is involved in the investigation of the collective processes emerging when a system is driven out of thermodynamic equilibrium condition. As a collateral activity he is involved in the development of instrumentation for material investigation. As an example, he was the leader of the Italian team which designed and built the energy selective neutron tomography device now installed at the IMAT beam line of ISIS (STFC, UK) and officially inaugurated on October 10, 2016. Actually he take the position of Research Director at IPCF-CNR, Messina, Italy.

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### Notes:



11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Co-electrodeposition of Zn-rich Cu-Zn-Sn metallic alloy and its conversion to $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{ZnSnSe}_4$ photovoltaic absorber films

AE Rakhshani, F Al-Sagheer, A. Bumajdad, S Thomas and PH Tharayil  
Kuwait University, Kuwait

$\text{Cu}_2\text{ZnSnS}_4$  (CZTS) and  $\text{Cu}_2\text{ZnSnSe}_4$  (CZTSe) compound semiconductors are promising absorber materials for thin film solar cells due to their intrinsic p-type conductivity, high optical absorption coefficient, and suitable band gap energy. Furthermore, these absorber films are composed from the abundant and non-toxic elements. Among different techniques which can be used for the preparation of these two absorber layers, solution processed techniques are very attractive due to their simplicity and low cost advantages. Here, we report the results of our study on the co-electrodeposition of a Zn-rich precursor metallic alloy Cu-Zn-Sn film from a single water-based solution with a composition not previously reported. The precursor films were converted to CZTS and CZTSe by vapor phase sulfurization and selenization processes. The synthesized films were characterized for their surface morphology and structure by using scanning electron microscopy (SEM) and X-ray diffraction (XRD), respectively. Raman spectroscopy was employed for the identification of films and the detection of impurity phases which could exist. Photocurrent spectroscopy was used to measure the films optical transition energies, including the band gap energy. Heterojunction CdS/CZTS and CdS/CZTSe devices with the typical diode-type current-voltage characteristics could be prepared and their device parameters were evaluated. The results revealed that device-quality absorber films can be synthesized successfully by co-electrodeposition from a single bath solution used in this study.

### Biography

Ali Rakhshani is an educator and researcher working at Kuwait University (department of Physics). He obtained his PhD and MTech degrees in the field of Semiconductor Physics and Technology from Brunel University (UK) and BSc degree in Physics from Tehran University (Iran). He gained his postdoctoral research experience on photovoltaic devices in Wayne-State University (USA) and in Queensland University (Australia). His research expertise is in the field of thin film semiconductor materials and devices with orientation towards the synthesis of thin optoelectronic films and the fabrication of related devices. He and his collaborators are currently working on the development of solution-grown light absorber films for photovoltaic applications.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Surface mechanics design of metallic materials by cavitation peening

**Hitoshi Soyama**

Tohoku University, Japan

Cavitation normally causes damage in hydraulic machineries such as pumps and screw propellers, as severe impacts are produced at cavitation collapses. However, cavitation impacts can be utilized for surface mechanics design for improvement of fatigue strength in the same way of shot peening. The peening method using cavitation impacts is named as “cavitation peening”. The advantage of cavitation peening is that the increase of surface roughness is small comparing with conventional shot peening, as shots are not required in cavitation peening. In order to mitigate stress corrosion cracking, introduction of compressive residual using cavitation impact was proposed, and it has been applied for nuclear power plants. By enhancing cavitation impacts, improvement of fatigue strength was demonstrated. The aspect of cavitation peening of gear by using a submerged water jet with cavitation, i.e., a cavitating jet. In order to investigate mechanism of improvement of fatigue strength, a special fatigue tester was developed to investigate crack propagation in surface modified layer. Cavitation peening also suppress hydrogen embrittlement. At laser peening, it is believed that impact caused by laser abrasion produces plastic deformation for surface treatment. However, a bubble is generated after laser abrasion, and it produces impact at bubble collapse like cavitation, then it can be called as laser cavitation. As shown in Fig. 2, when the impact passing through the material was measured, the impact induced by laser abrasion is larger than that of laser abrasion. Namely, at submerged laser peening, peening effect would be improved by considering the laser cavitation. In the presentation, the principal of cavitation peening is introduced with applications of cavitation peening such as improvement of fatigue strength and suppression of hydrogen embrittlement. The work was partly supported by Osawa Scientific Studies Grants Foundation.



**Figure2:** *Laser abrasion and laser cavitation at submerged laser peening by a cavitating jet*

### Biography

Hitoshi Soyama is Professor of Department of Finemechanics at Tohoku University, Japan. He is a Fellow of American Society of Mechanical Engineers ASME and a honorary member of Water Jet Technology Society of Japan. 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. He established evaluation methods using inverse analysis to investigate mechanical properties of surface modified layer. Now, he has been applied the evaluation methods to mechanical properties of products of additive manufacturing. He proposed additive manufacturing of laser melting using oxide iron on Mars and/or Moon. It was revealed that oxygen was obtained during the process.

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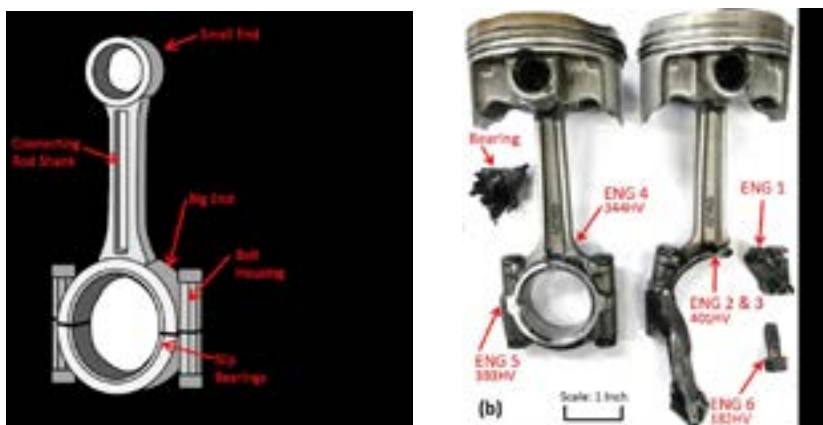
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Fatigue analysis of a failed connecting rod in race car engine

K. Bari<sup>1</sup>, A. Rolfe<sup>1</sup>, A. Christofi<sup>1</sup>, C. Mazzuca<sup>1</sup> and K.V. Sudhakar<sup>2</sup><sup>1</sup>University of Derby, United Kingdom<sup>2</sup>Montana Tech of the University of Montana, USA

In the present work, a failed connecting rod from a motorcycle engine was investigated for the root cause of and possible mechanisms leading to its premature failure. In addition to finding the root cause, the expectation from this study was to possibly improve the existing designs or practices to avoid similar failures in future. These results were validated using a finite element analysis (FEA) simulation. A Scanning Electron Microscope was used for investigating the mechanisms of fracture modes, optical microscopy for studying the microstructures and visual inspection were primarily utilized to determine the root cause of the failure. In conclusion, it was determined that the root cause for the premature failure of the connecting rod was the presence of scale build-up inclusions, which led to micro cracking during fatigue loading of the component. It is most likely that the connecting rod failed on the end of exhaust stroke, due to the tensile force being at its highest, when the piston reaches TDC. This is due to the inertia of the piston, pin, and upper end of the connection rod moving upwards while there are no compressive forces to take them under consideration.



**Figure1:** (a) Diagram of an assembled connecting rod, rod cap, bolts and slip bearing with key features and components annotated in red; (b) The intact and failed connecting rod and piston assemblies, left and right consecutively, are shown with the failure.

### Biography

Dr. Klaudio Bari is a senior Lecturer at University of Derby. He has passion for fatigue in engine component, in particular race car, that endure stress, heat and corrosion environment at the same time. Stress crack corrosion is a complex subject and can be only understood after comprehensive analysis in term of using scanning electron microscope and particular mode (EBSD). In general, visual analysis can be helpful sometime, but often is misleading the fact and lead the investigator to wrong conclusion. Conservative approach in failure analysis is definitely his strong point in Engineering.

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### Notes:

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Crack/Damage evaluation and micro-materials fabrication in the relation with electric field

**Masumi Saka**

Tohoku University, Japan

Evaluation of materials subjected to electric current and Joule heating has been studied by many researchers and fruitful results have been reported. In my presentation, crack problems in a conductive material are first discussed. The path-independent integral for an electric crack problem in a plate subjected to current is explained with its relations to Joule heating near the crack tip and the increase in electric resistance of the plate due to a unit crack extension. Regarding nondestructive evaluation of cracks, highly sensitive direct current potential drop technique, that is closely coupled probes potential drop (CCPPD) technique, is explained with its principle and superior characteristics for evaluation of closed cracks. Also evaluation of multiple cracks is mentioned. In the second, a topic in the field of micro and nano materials evaluation is explained, which is a subject of electrical failure of a metallic nanowire mesh due to Joule heating. Characteristic nature of sequential melting of nanowires in the mesh is explained for respective conditions of current control and voltage control. Next, electromigration (EM) phenomenon, which is atomic diffusion due to electron flow in high density, in metallic thin-film materials related to reliability of integrated circuits is discussed, where the effect of passivation on damage suppression is focused. Finally, fabrication of micro materials of wire and sphere is explained as utilization of EM, where the effect of temperature caused by Joule heating on the shape of formed micro material is mentioned. In addition, the other phenomena of atomic migration such as stress migration and ionic migration are discussed in comparison with EM from a few points of view. Electric field and Joule heating are connected with materials science and evaluation on many equipments, machines and structures. As written above, four topics related to these physical quantities are reviewed in this presentation.

This presentation is supported by JSPS KAKENHI Grant-in-Aid for Scientific Research (B) No.17H03139.

### Biography

Masumi Saka received his Bachelor of Engineering degree in 1977 and his Doctor of Engineering degree in Mechanical Engineering in 1982, both from Tohoku University, Sendai, Japan. He became a Professor at Tohoku University in 1993. His research interests lie in the evaluation of materials system and the fabrication of metallic micro- and nano-materials. He is Editor of a book entitled "Metallic Micro and Nano Materials".

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

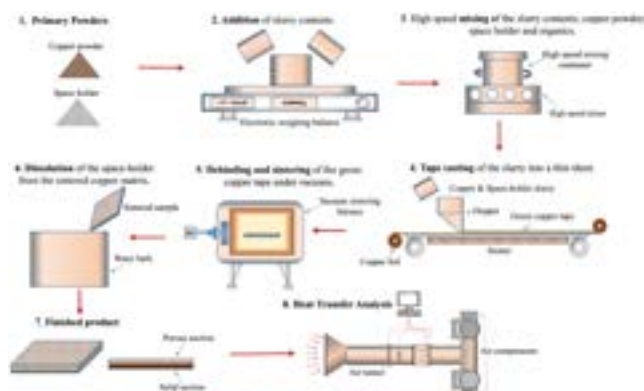
## Heat transfer performance of double-layer porous copper produced by tape casting with lost carbonate sintering

Mosalagae Mosalagae<sup>1</sup>, Ahmed AAG. Al-Rubaiy<sup>2</sup>, Russell Goodall<sup>1</sup> and Robert Woolley<sup>2</sup>

<sup>1</sup>Department of Materials Science and Engineering, University of Sheffield, UK

<sup>2</sup>Department of Mechanical Engineering, University of Sheffield, UK

Porous copper tapes with high surface area to thickness ratio are attractive for thermal management in portable electronics where good heat transfer performance is required. In this study, the porous sheets of thickness down to  $1350\mu\text{m}$  were investigated for heat transfer performance. The porous copper samples were produced by a novel process combining lost carbonate sintering (LCS) and tape casting. This process allows the flexibility to produce copper double-layer structure consisting of a porous section with a wide range of porosities on a dense substrate. Here double-layer structures consisting of a porous layer of porosities ranging from 30-70% were investigated. Their suitability for heat sink applications were investigated with simple assessments of the thermal properties under forced convection using air as a coolant. Through experiments, the heat transfer performance of the thin porous tapes was systematically studied under two different heating systems; a cylindrical and flat heating systems. The heat generated within the heating systems was controlled by AC/DC power supply. Also the flow rate of air passing through the samples was varied between the ranges of 0 – 0.5 kg/s. T- type thermometers and an Infrared thermography sensor were installed in the system to track in and out and surface temperatures of the system. This allowed behavior of heat dissipation by porous copper tapes to be effectively studied. The initial experimental results showed that, from the thermal viewpoint, the porous copper heat sinks investigated here have an excellent heat transfer performance. The outcome of this study is fully discussed in the presentation.



**Figure1** Schematic diagram showing processing and heat transfer analysis of porous copper samples

### Biography

Mosalagae Mosalagae is a professional, highly motivated and dedicated materials science and engineering researcher. His main interest is on development of porous metals for heat transfer applications by powder metallurgical processes. He developed a process which combines lost carbonate sintering (Zhao et al, 2004) and tape casting to process copper powder into thin sheet of porous copper, and further developed a heat transfer rig to investigate the porous heat sinks produced by simple assessment of thermal properties. In this rig, porous metals are tested under a forced convection using air as a coolant.

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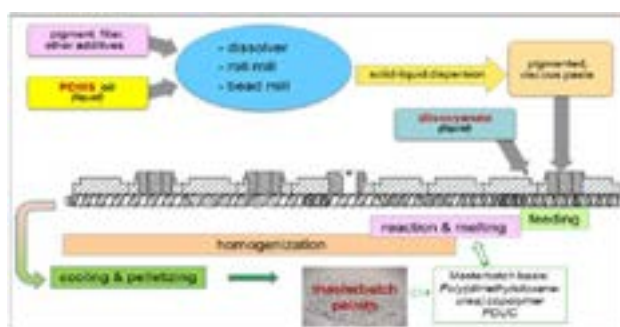
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Advanced poly dimethylsiloxane-urea copolymer based masterbatches with multiple functionality

Hans-J. Radusch<sup>1</sup>, Matthias Huebner<sup>2</sup>, Friedhelm Roeber<sup>2</sup>, André Wutzler<sup>3</sup> and Nadine Poenisch<sup>4</sup><sup>1</sup>MLU Halle, Germany<sup>2</sup>DAW Nerchau, Germany<sup>3</sup>PSM Merseburg, Germany<sup>4</sup>KUZ Leipzig, Germany

Optical and esthetic modification is a basic need for polymer application in all technical and consumer fields. Colorants are used in broad volume to satisfy the demand of costumers for that purpose. Organic or inorganic colorants are included in a carrier polymer, which should help to dose the colorant precisely, to mix it homogeneously, to be compatible with the matrix, and it should not influence the mechanical and rheological properties unfavourably. A colorant masterbatch on the basis of polydimethylsiloxane-polyurea copolymer (PDUC) was developed. The masterbatch was generated by an innovative processing technology coupling a pre-dispersion step and a fluid component based reactive extrusion step. A specific twin-screw extruder with feeding units is used for the liquid initial components polydimethylsiloxane (PDMS) including the pre-dispersed colorant as well as the diisocyanate. The precise stoichiometric ratio of the components as well as the optimization of residence time of the polymer in the extruder in concern to the reaction time of the components allowed the generation of the PDUC based masterbatch. Different isocyanates and aminopropyl terminated PDMS were used. A higher number of thermoplastics was involved into the investigation of the suitability of the generated masterbatches. Beside the nearly universal applicability of the masterbatch, the improvement of processibility - expressed by lowering of the viscosity, reduction of energy consume of the extruder or reduction of rejection forces at injection molding - could be demonstrated. Thus, the masterbatch proves to be not only an effective colorant, but also an internal lubricant. The good dispersion of the pigment particles was demonstrated by optical microscopy. Stress-strain measurements proved that no significant negative influence of the new masterbatch in concentrations < 5 % on the mechanical properties of the investigated thermoplastics could be observed. Furthermore could be shown that the masterbatch composition and manufacturing technology is suitable as carrier for the inclusion of nano-particles into polymer materials.



**Figure1:** Masterbatch generation by coupled dissolver pre-dispersion and reactive twin-screw mixing technology.

### Biography

Hans-Joachim Radusch is an expert in the field of the development of new polymer materials by blend and composite technologies under special consideration of nanofillers and nature based polymers. He graduated with a PhD thesis in the field of polymer processing in 1975. After his PhD study, he was employed in industry before he returned to Technical University Merseburg, where he habilitated with a thesis on polymer blends in 1985. 1989 he became a professor of Polymer Materials Technology at the Technical University Merseburg, and 1994 he was called for a full professorship for Polymer Technology at the Martin Luther University Halle-Wittenberg. Since more than 30 years he has a lot of experience in modification of polymers by reactive polymer processing as well as polymer materials characterization.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Sculpture art and fashion design

Maryssa El Fare and Nashwa El Shafey  
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For thousands of years sculpture has conducted many roles in human life. The Greeks made statues that depicted perfectly formed men and women with their beauty and elegant dresses. Early Christians decorated churches with acanthus leaves, where this pattern revealed a good motive and inspiration to the fashion designers. Egyptian artists used a wide array of materials, the lotus blossom carved on their temple and its pillars, so the fashion designers copied that sculpted to their dresses. For instance, already in the ancient Egyptian garments, it was decorated by repeating the pattern of lotus blossom. The beauty and elegance of the paisley leaf has inspired artists, architects and craftsmen for centuries since it was sculpted at the Persian age. Among fashion designs makers, printing this classic detail in their dresses. From the beginning of century until the present, sculpture has been largely a very inspired monumental. In the 15<sup>th</sup> century, monuments to biblical heroes were built on the streets of Italian cities with their formal dress. The Italian fashion designer inspired their fashions from the great fountain with acanthus leaves sculpture in the centre of the cities. However its vary so greatly in style and shape where they are sometimes difficult to identify as an acanthus leaf. The beauty and elegance of the acanthus leaf has inspired artists, architects and craftsmen for centuries as shown on the US capital building as its The present research is dealing with the relationship between sculpture and the art of fashion design as inspiration from different Civilisation and centuries pillars has decorated with acanthus leaves as well as the fashion designers inspired their dresses now days. The Figure is showing the acanthus leaves decorated sculptured pillar (top) and the inspired fashion design dress (bottom).



## Biography

Maryssa Elfare is expert in sculpture different materials Clay granite, polyester and Wood. Have different galleries on the level of faculty of applied arts and university and interested in fashion design.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Material science and fashion design

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Technology is changing life so dramatically whilst globally, textiles represent the fourth largest manufacturing industry, with the apparel sector forming the most valuable component of this industry. Garment design is an integration of all the advanced design elements including colour, texture, space, lines, pattern, silhouette, shape, proportion, balance, emphasis or focal point, rhythm and harmony. The more advanced the technology involved, the more forward-thinking fashion will be. However the new technique of printing fabric digitally is to textiles as 3D printing as product manufacturing. The slow process of fabric printing designers is used to upgrading, allowing them to create things more quickly. Differently Style of Architecture- fashion paper-engineering inspired garments with folded fabric cut outs; 3D fashion. Different technology as material metaphor is the unifying theory of a rationalized space and a system of motion. The material is grounded in tactile reality, inspired by the study of paper and ink, revealed technologically advanced and open to imagination and magic. Austrian architect Julia Körner, who collaborated with Van Herpen on the digitally fabricated garments, into everyday clothing production as part of what she calls an "exciting moment in fashion design". Architecture Julia Körner created the advances in 3D scanning, modeling and printing as a revolution in customized fashion pieces within ready to wear. The present research is focusing on designers who are introducing the advanced technological fashion world to new technologies where to cover our bodies for protection where it came before the desire to decorate ourselves fashionably, initially from the elements and eventually from each other in a fashionable trend.



## Biography

Nashwa El Shafey (Prof.Dr. assistant) is expert in fashion design and has established several fashion shows on the level of the faculty of applied arts and University- the author of the book of fashion theories(under publishing)

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September 07-08, 2017 | Edinburgh, Scotland

## Structures, interactions and optical responses from polymer and polymer nanocomposites

**Sarathi Kundu**

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Biological functions of biopolymers like proteins strongly depend upon their structures which can be modified by the interactions with surrounding environments. Understanding protein-protein interactions in solutions are very important as it helps in obtaining protein crystals, biochemical roles of proteins, ideas about some diseases like Alzheimer, Parkinson, etc. Biochemical functions of proteins are regulated in the presence of ions around them and hence the effect of ionic strength, nature of ions, temperature, pH, concentration, nanoparticles, etc. strongly affect the protein-protein interactions. Among different proteins, globular proteins like BSA, HSA, lysozyme can be considered as charged, colloidal particles and both short-range attraction and long-range electrostatic repulsion exists among the protein molecules in solution and hence Derjaguin-Landau-Verwey-Overbeek (DLVO) potential can be applied to obtain the interaction nature and to explain the phase behaviors. However, DLVO model cannot fully explain the rich behavior of proteins due to the presence of inhomogeneous surface charges and irregular shape of proteins. One, two or three attractive or repulsive Yukawa form potentials were also used to explain the nature of interactions. Small angle neutron scattering (SANS) study shows that in combination with the short-range attraction and intermediate-range electrostatic repulsion, a possible weak long-range attractive interaction between protein molecules may exist. SANS study also shows that for different counterions and for the equal ionic strength, the interactions are largely modified by the tri-valent ( $\text{Fe}^{3+}$ ) and di-valent ( $\text{Ni}^{2+}$ ) ions and comparatively less by the mono-valent ( $\text{Na}^+$ ) ions. Below the isoelectric point, protein has a net positive surface charge although local charge inhomogeneity presents and as a result interaction nature modifies. In presence of different ions, cold gelation behaviors of proteins have also been studied which indicates the fractal structure formation after gelation. In presence of charged polymers, conformational changes of globular proteins may occur depending upon the charge states of the polyelectrolytes. Protein-polyelectrolyte complexes (PPC) show modified behaviors than that of pure protein/polymer. It has been observed that the thin films of PPC show a larger red-shift in the fluorescence emissions in comparison with that of pure protein. Protein and protein films are also used as templates to form metallic nanostructures of different shapes and sizes which are also used for modifying both optical and electrical properties.

### Biography

Dr. Sarathi Kundu did his M.Sc. from Visva-Bharati University, West Bengal. He completed his Ph.D. work from Saha Institute of Nuclear Physics, Kolkata in 2006 and the degree is conferred by Jadavpur University. He did his Post-Doctoral research work from University of Paris Sud, France. He was Visiting Faculty Fellow in S.N. Bose National Centre for Basic Sciences, Kolkata and Visiting Scientist in KEK, Japan. At present he is Associate Professor in IASST, Guwahati. Dr. Kundu has been working on soft matter physics with emphasis on organic thin films and nanomaterials. He is interested to explore structures and properties using scattering, spectroscopic and microscopic methods. Dr. Kundu has published nearly 50 journal papers so far.

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## Recent advances in polylactic acid based blends, composites and nanocomposites for packaging and barrier applications

Kartikey Verma<sup>1,2</sup> and Babulal Chaudhary<sup>1</sup><sup>1</sup>Chandigarh University, India<sup>2</sup>Indian Institute of Technology, India

Development of biodegradable materials is highly in demand as large and rapid usage of plastic materials results million tons of plastic wastes in the landfill sites each year globally. It takes a long time for conventional plastics to degrade, leading to severe ecological problems too. The production capacities of biodegradable plastics, such as polylactic acid (PLA), polyhydroxyalkanoates, and starch blends, are also growing steadily, nearly doubling from 0.7 million metric tons in 2014 to well over 1.2 million metric tons by 2019. PLA, for its good compatibility and biodegradability, is preferred by people from all sectors. Also, PLA is a low energy consumption product, about 30-50% lower in energy consumption than the petroleum-based polymers. PLA as the most widely used, the lowest price of bioplastic in industrialization, in the aspect of practicality, is the biodegradable material that has the largest scope to replace the position of the petroleum based plastics on the current scenario of oil scarcity. The production cost of PLA is also approaching the cost of traditional plastic, and with the strong expansion of market applications, will get soon recognized globally. PLA based nanocomposites are widely used today in various applications. The review article aims to target on the topical progresses in the synthesis and characterization of PLA blends, PLA composites and PLA nanocomposites with different materials. Moreover, this article is a unique collection of vital information about PLA based blends and composites for drug delivery, packaging and barrier applications in a single platform.

### Biography

Dr. Kartikey Verma is working as professor in Indian Institute of Technology, Roorkee, India. His research interest is on advanced materials, biomaterials, Nanotechnology.

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September 07-08, 2017 | Edinburgh, Scotland

## Scientific Tracks & Abstracts Day 2

Advanced Materials 2017

# Sessions:

Day 2 September 08, 2017

## Materials Engineering and Performance | Materials For Engineering and Environmental Sustainability | Polymers Science and Engineering | Optical, Electronic and Magnetic Materials

### Session Chair

**Nekane Guarrotxena**

CSIC, Spanish National Research Council, Spain

### Session Chair

**Sylvain G. Cloutier**

École de Technologie Supérieure, Canada

### Session Introduction

**Title: Adsorptive removal of sulfur compounds using Cu<sup>2+</sup>-based porous coordination polymers**

**Masashi Morita**, Panasonic Corporation, Japan

**Title: Key role of the liquid-surface interactions to reveal hidden elastic properties in liquids**

**Laurence Noirez**, Université Paris-Saclay, France

**Title: Influence of nickel and aluminum additions on the microstructure and tensile properties of innovative, free-carbon, 10% cobalt maraging composite steel**

**Saied Elghazaly**, Central metallurgical R&D Inst, Egypt

**Title: Functionalized well-defined polymeric nanostructures for biomedical applications**

**Efrosyni Themistou**, Queen's University Belfast, UK

**Title: The performance of polypropylene fibre reinforced concrete: Mechanical properties**

**Noor Faisal Abas**, Universiti Sains Malaysia, Malaysia

**Title: Polymeric nanoparticles and gels: Modeling of dynamic behavior and properties using Discrete Element Method**

**Martin Kroupa**, University of Chemistry and Technology Prague, Czech Republic

**Title: High-performance perovskite hybrids for printable optoelectronics**

**Sylvain G. Cloutier**, École de Technologie Supérieure, Canada

**Title: Hydrogen production from water using the sun via photocatalytic processes on Au/g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> materials**

**Valerie Keller**, Institute of Chemistry and Processes for Energy, Environment and Health, France

**Title: On unified approach in description of crystalline structures in discrete space**

**Vladimir Shevchenko**, Institute of Silicate Chemistry RAS, Russia

### Video Presentations

**Title: Engineering columnar crystals: A novel, template-based method of sequential deposition**

**Ho-kei Chan**, Harbin Institute of Technology, China

**Title: Microstructure development affected by electrode geometry during resistance spot welding**

**Peng-Sheng wei**, National Sun Yat-Sen University, Taiwan

11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Adsorptive removal of sulfur compounds using Cu<sup>2+</sup>-based porous coordination polymers

Masashi Morita<sup>1</sup>, Hidenobu Wakita<sup>1</sup>, Takaiki Nomura<sup>1</sup>, Yoichiro Tsuji<sup>1</sup>, Masakazu Higuchi<sup>2</sup> and Susumu Kitagawa<sup>2</sup><sup>1</sup>Panasonic Corporation, Japan<sup>2</sup>Kyoto University, Japan

Adsorptive removal of toxic substances is of crucial importance both in industry and in living environments. In general, porous materials such as zeolites and activated carbons are used as the adsorbents. Ag-Y zeolite is widely used for the adsorptive removal of sulfur compounds from natural gas at ambient temperatures in fuel cell cogeneration systems in spite of its low adsorption capacity and high cost. For the purpose of a more efficient and simple process, new types of porous materials for adsorbents are strongly required. In recent years, porous coordination polymers (PCPs) or metal-organic frameworks (MOFs), which have high surface areas and act as molecular sieves owing to their micropores have been studied due to their potential applications in gas storage, molecular separation and catalysis. PCP/MOFs, as adsorbents, offer the advantages of having high surface area, ordered structures, and adjustable chemical functionality. The unique adsorptive reactions of various materials have been reported. Herein, we applied porous coordination polymers (PCPs) to adsorbents for the removal of sulfur compounds and also investigated how the metal ions highly dispersed in PCPs affected the adsorption capacity and how the open metal sites functioned as the adsorption sites. HKUST-1, which is composed of Cu (II) and trimesate, was examined to remove methanethiol (MT) from hydrocarbon gas at 30 °C. As a result, HKUST-1 showed high sulfur adsorption capacities for MT (8.4 wt.%), compared with those on Ag-Y zeolite (3.0 wt.%). Spectroscopic study revealed that a MT was adsorbed on Cu (II) site to produce a dimerized dimethyldisulfide (DMDS) accompanied by a reduction of Cu (II) to Cu (I). To conclude, we have utilized HKUST-1 for the adsorptive removal of MT from hydrocarbon gas. It was experimentally shown that highly dispersive Cu (II) sites in HKUST-1 are effective for the removal of sulfur compounds.

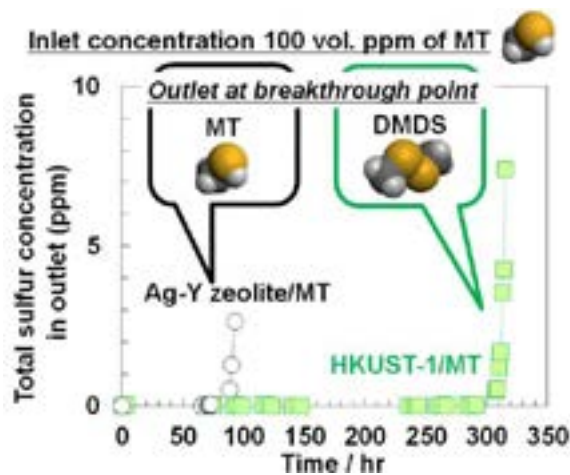


Fig1: Breakthrough curves of total sulfur concentration for MT adsorption

### Biography

Masashi Morita was born at Saitama, Japan, in 1988. He received his B.Sc. and M.Sc. degrees from Waseda University in 2011 and 2013 respectively under the direction of Professor Makoto Ogawa. He joined in Research & Development division, Panasonic Corporation as a researcher, in 2017, he became a senior researcher. His research interests include the synthesis and applications of porous materials towards the adsorbents and catalysts.

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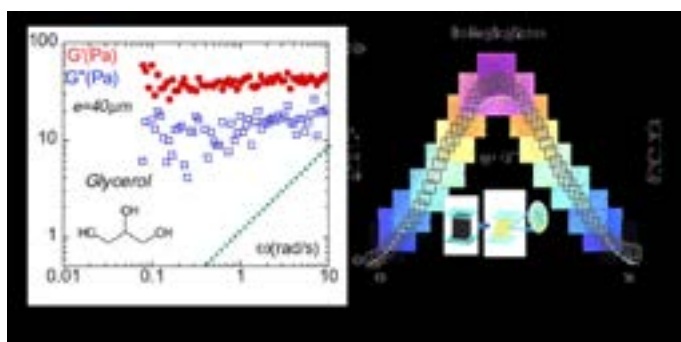
September 07-08, 2017 | Edinburgh, Scotland

## Key role of the liquid-surface interactions to reveal hidden elastic properties in liquids

**Laurence Noirez**

Paris-Saclay Université, France

At the liquid-solid interface, the energy of the liquid is different from the bulk due to the imbalance between the attraction forces between molecules (cohesion) and the interactions of the molecules to the surface (wetting). In case of ceramic composites, liquid molecules are so strongly attracted to the high energy surface that the surface procures a total wetting. Because the viscosity measures the energy necessary to transfer a motion from a surface to the liquid, the force of the interactions to the substrate plays a key role in the determination of the fluid properties. By improving the liquid/surface boundary forces, high energy surfaces optimize the motion transfer during the rheological measurement. Low frequency shear elasticity becomes measurable bringing robust evidence that liquid molecules are not dynamically free but elastically correlated. The elastic property is experimentally identified on polymer melts, glass formers, Van der Waals liquids or liquid water pointing out a generic property. It sheds a new light on the mechanisms that govern liquid transport, gelation or glass processes or active materials and allows the identification of new effects as the conversion of a liquid phase in a strain-driven optical harmonic oscillator or the production of cold under flow that become possible when the liquid molecules are strongly anchored on high energy substrates.



a) By improving liquid/substrate boundaries, glycerol reveals a solid-like response at the mesoscopic scale (measured at room temperature, 40 $\mu$ m thickness).

b) New effects as the conversion of a liquid phase in an opto-mechanical oscillator are revealed and visualize the elastic response (thickness 200 $\mu$ m).

### Biography

Dr. Laurence Noirez is CNRS Research Director at the Laboratoire Léon Brillouin (LLB), Université Paris-Saclay (France). She is working in a large facility that welcomes around 500 experimentalists per year; Dr. Noirez has a 25 years expertise in neutron scattering, diffraction and instrumentation. Her main developments concern a multiscale structural and dynamic study of simple and complex fluids (microfluidics) taking into account in particular the liquid/surface boundary conditions. Dr. L. Noirez established that liquids are long range elastically correlated and measured their low frequency shear elasticity. She also evidenced the impact of the interfacial forces on the liquid flow showing in particular that liquids can produce cold. She has published over SCI 130 articles.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Influence of nickel and aluminum additions on the microstructure and tensile properties of innovative, free-carbon, 10% cobalt maraging composite steel

Saied Elghazaly<sup>1</sup>, Waleed Elghazaly<sup>1</sup>, Omyma Elkady<sup>2</sup> and Sabine Weiss<sup>3</sup><sup>1</sup>Steel Technology Lab, CMRDI, Egypt<sup>2</sup>Powder Metallurgy Lab, CMRDI, Egypt<sup>3</sup>TU Cottbus, Germany

Good combinations between strength and toughness are always the aim of all researchers working in the field of material science. Maraging steel grades (200-300) are one of the well known steel alloys proved to have good strength and toughness and are known as 18%Ni-Co-Mo steel family. Maraging steels production, import, and export by certain countries such as USA is closely monitored by international authorities because it is particularly suited for use in gas centrifuges used for uranium enrichment and in aviation technology. In this research an effort is paid to produce innovative carbon-free maraging steel alloy composites that can compete the well known 18%Ni-8%Co standard (250-300) maraging steel alloy with higher strength and superior toughness. The experimental maraging steel composites having different Ni (18-25%)-and Al (0.5-1.5%) together with or without Ti and Mo contents are produced by consolidation from the nano-elemental powders. The mechanism of strengthening in Iron- Nickel- Cobalt-Aluminum composite alloys is studied, however, the changes in microstructures after solution treatment and aging-heat treatment are emphasized using metallurgical microscopy and SEM-TEM aided with EDX analyzing unit. The effect of induced deformation on the properties of the as-sintered samples is also studied. Fracture toughness, impact toughness, hardness, and strength are measured for all alloy composites under investigation and compared with the standard nominal properties for conventional maraging series (250-300).

### Biography

Prof. Dr. Saied Elghazaly is working with steel technology group at the central metallurgical R&D Institute, Cairo-Egypt since 1974. He has a wide experience in the field of steel alloys especially stainless, tool, and high alloy steels produced through conventional or powder metallurgy routes.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Functionalized well-defined polymeric nanostructures for biomedical applications

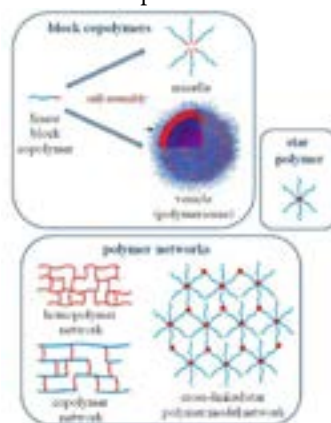
Efrosyni Themistou, Thomas J. Gibson and Marie Finnegan  
Queen's University Belfast, UK

**Statement of the Problem:** Novel polymers bearing functional groups are essential in various biomedical applications. Biocompatible polymeric nanostructures including star polymers and amphiphilic block copolymers that self-assemble to polymer micelles and vesicles in aqueous solutions, enable the intracellular delivery of hydrophobic and hydrophilic drugs, antibodies, proteins and DNA, without affecting cell metabolic activity. Amphiphilic block copolymers can be also used for the functionalization of nanofibers for tissue engineering applications. The purpose of this study is to explore the preparation of biodegradable star polymers and amphiphilic block copolymers using reversible addition-fragmentation chain transfer (RAFT) polymerization and ring opening polymerization (ROP).

**Methodology & Theoretical Orientation:** For the synthesis of the amphiphilic block copolymers the biocompatible water-soluble poly [2 (methacryloyloxy) ethyl phosphorylcholine] (MPC) and oligo(ethylene glycol) methacrylate (OEGMA) monomers were used for the formation of the RAFT macro- chain transfer agent (CTA). Various hydrophobic monomers were used for the efficient chain extension of these macro-CTAs, leading to the formation of amphiphilic block copolymers (either by RAFT polymerization or ROP). For the preparation of star polymers by aqueous RAFT polymerization, a degradable acetal-based cross-linker was used to connect the hydrophilic macro-CTA linear chains together to form star-shape polymeric nanostructures. All polymers were characterized by NMR and GPC, where the formation of the polymeric nanostructures, achieved either by self-assemble methods or chemical cross-linking, was indicated by TEM and DLS studies.

**Findings:** RAFT polymerization and ROP are great methods for producing well-defined polymeric nanostructures. Thin film rehydration, pH-switch, solvent-switch and polymerization-induced cell-assembly (PISA) can be used for the formation of various polymer morphologies in aqueous solutions (micelles and vesicles), which are important for biomedical applications.

**Conclusion & Significance:** The polymers prepared in this work are currently being evaluated for site-specific delivery of biologically important molecules, as well as for their use as protein sensors and tissue engineering matrices.



**Figure:** Polymeric nanostructures prepared by 'Living' polymerization techniques

### Biography

Dr. Efrosyni Themistou is a chemical engineer with a PhD in Polymer Chemistry. She worked as a Post-doctoral research associate in the University of Cyprus, the State University of New York (SUNY) – University at Buffalo, USA and the University of Sheffield. She became a Lecturer in Materials in the School of Chemistry and Chemical Engineering at Queen's University Belfast, UK in 2013. Her current research is on the synthesis of well-defined polymeric materials using various advanced polymerization techniques. Techniques such as NMR, GPC, DLS, TEM, SEM and SAXS are used to characterize these materials. These polymers can find various applications as drug/protein/DNA delivery vehicles, sensors and tissue engineering matrices.

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11<sup>th</sup> International Conference on

# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## The performance of polypropylene fiber reinforced concrete: Mechanical properties

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This paper investigated the mechanical properties of polypropylenes fibers on normal concrete. Effects of addition polypropylene fiber on concrete are studied. Polypropylene fiber act as additives by volume. This research are conduct with three different type of mixing where each of mix containing different percentage of polypropylene fiber that are 0.3%, 0.6% and 0.9%. Compression test, flexural test and water absorption test were carried out to determine the mechanical properties. All tests are conduct by using a standard method of testing. The different type of mixing has been tested with different aged 7, 14, 21 and 28 days. The overall specimen that was prepared to tests is 48 cubes and 32 prisms. From the data obtained, results show that slightly increase in compressive strength. But, the higher the fibers content, the lower its strength. This research indicated that 0.3% fibers have higher result in compressive test while 0.9% higher in flexural strength. The lowest percentage of water absorption test is 0.3% with 5.19% at 28 days.

### Biography

Associate Professor Dr. Noor Faisal Abas is currently a senior lecturer at the School of Housing, Building and Planning, University Sains Malaysia, Penang, Malaysia. He has published his academic articles in indexed journals and presented many international and local papers in the field of engineering, building material and building construction. He is leading a few research projects on alternative building materials, cement replacement materials and fiber concrete. His area of expertise is building technology and construction material.

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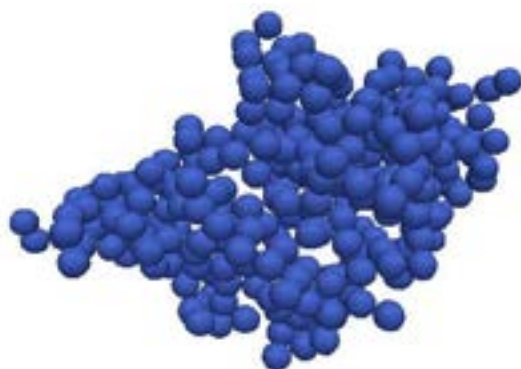
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Polymeric nanoparticles and gels: Modeling of dynamic behavior and properties using discrete element method

Martin Kroupa, Jose F. Wilson, Miroslav Soos and Juraj Kosek  
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Polymeric nanoparticles have a broad spectrum of applications including dispersion (emulsion) paints or thin films. However, the understanding of their behavior and properties, especially at high concentrations is still limited. We model the dispersions of polymeric nanoparticles using the dynamic model based on Discrete Element Method (DEM). The interaction model represents particles that are elastic, adhesive and electrostatically stabilized. The flow-field computation that is included in the model enables us to evaluate the rheological properties of the dispersion, which are crucial for its behavior. Further characterization of both dispersions and gels is done using oscillatory simulations, from which the viscoelastic properties are obtained. The model was successfully used to describe the dynamic behavior of a flowing dispersion including the processes of coagulation, fouling and breakage. These processes and their relative importance in a specific system determine the transition from a dispersed state to a gel. Due to their specific position on the boundary between solids and liquids, gels have unique properties that make them suitable to be used e.g., as a porous structures (or) matrices for drug delivery in the pharmaceutical industry.



**Figure1:** Colloidal aggregate produced by shear-induced aggregation. Result of a numerical simulation

### Biography

Martin Kroupa obtained his B.Sc. and M.Sc. at University of Chemistry and Technology Prague, Czech Republic. His research interests lie in the area of colloidal and interface science with the main focus on the dynamic behavior of concentrated colloidal dispersions and related phenomena such as coagulation and fouling. These phenomena are closely connected to the rheology and thus the modeling of rheological behavior is another large area of interest of M.K. He is also active in the field of electrochemistry.

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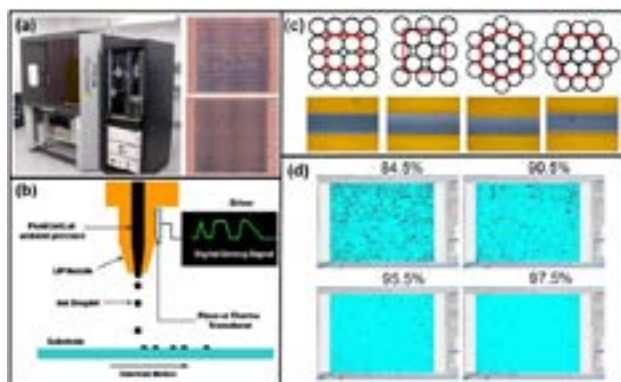
September 07-08, 2017 | Edinburgh, Scotland

## High-performance perovskite hybrids for printable optoelectronics

Sylvain G. Cloutier

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In the last 5 years, methylammonium lead halide or MALH perovskites (e.g.,  $\text{CH}_3\text{NH}_3\text{PbA}_{3-x}\text{B}_x$ , where A and B are I, Cl or Br) have shown tremendous potential for low-cost optoelectronic device integration, including light-emitting diodes, solar cells and photodetectors. For example, the power-conversion efficiencies from organometallic halide perovskite solar cells have increased from 3.8% in 2009 to 22.1% in 2016. This spectacular progress is largely attributed to improved processing and longer charge-carrier lifetimes, directly related to increased material quality. While significant progress was made, many key parameters including compatibility, interface engineering, surface treatment and processability remain essential to achieving the best device performances. These fundamental challenges prevent integration into commercial-grade devices. For one, relatively low carrier mobilities still prevent large-area devices with performances competing with state-of-the-art technologies. Several groups began exploring hybrid perovskite films in the last 3 years. In the last year, we have made major progress towards viable MALH devices (1) by dramatically enhancing structure and properties through solvent engineering, (2) enhancing conductivities by several orders of magnitude using MALH hybrids, (3) extending their operation to the near-infrared and (4) significantly improving their stability and lifetime by doping with SCN. Preliminary results shown in Fig.1 are greatly encouraging and suggest that the carefully-controlled processing capability allowed by the Ceradrop inkjet printer can yield high-quality MALH films. This is a major step towards the integration of MALH perovskites within commercial printable photovoltaic devices, LEDs and sensors.



**Figure:** (a) Commercial research-grade inkjet printer. (b) Unique control of the nozzle speed, temperature and drive signal can help optimize the jetting process.

(c) The splat pattern and the overlap ratio also have dramatic consequences on the printed features' quality.

(d) Fully-converted  $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$  (also called  $\text{MAPbI}_{3-x}\text{Cl}_x$  or MALH) nanocrystalline perovskite films printed with the printer. The control of the jetting helps optimizing the coverage and quality.

### Biography

Sylvain G. Cloutier received the outstanding Ph.D. thesis award in 2006 from the Division of Engineering at Brown University, where he studied the optoelectronic properties of nanoengineered materials. As an assistant professor of Electrical and Computer Engineering at the University of Delaware, he received the DARPA Young Faculty Award for his work on the use of Nano-engineered materials for lasers. In 2011, he joined ÉTS as professor of Electrical Engineering, where he leads the Canada Research Chair on Hybrid Optoelectronic Materials and Devices and explores new hybrid materials and heterostructures for optoelectronic device integration. He published more than 80 contributions cited over 1400 times and obtained 3 patents. In 2014, he was elected to the College of the Royal Society of Canada. At ÉTS, he is also the director of research, partnerships and faculty affairs.

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11<sup>th</sup> International Conference on

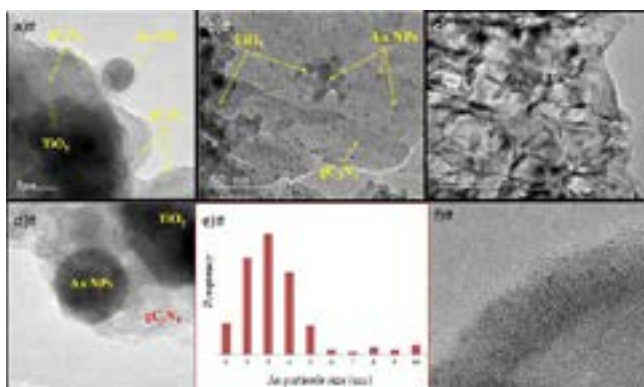
# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Hydrogen production from water using the sun via photocatalytic processes on Au/g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> materials

Valérie Keller, Clément Marchal, Pablo Calvo, Thomas Cottineau and Valérie Caps  
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The direct conversion of solar energy through an energy carrier (fuel), storable and usable upon request, appears as an interesting alternative to find environmentally friendly ways to produce energy. Photocatalysis is a promising way to produce hydrogen from renewable energy sources. Indeed, the water dissociation (water-splitting) highlighted by Fujishima and Honda in a photoelectrocatalytic cell opened a promising way to produce hydrogen from light energy. Since, many efforts have focused on the development of the water-dissociation in photoelectro- and photo- catalytic systems. Nowadays, one of the main challenges consist in the elaboration of semiconductor nanometaterials able to absorb visible-light wavelengths, to transfer efficiently the photogenerated charges, while keeping high stability of their performances under UV activation. For that purpose, different strategies are studied: Synthesis of semiconductors with narrow band gaps, doping (cationic, anionic, co-doping) approaches of wide bang gap semiconductors, heterojunction formation between wide- and a narrow band gap semiconductors for solar light harvesting, deposition of metal nanoparticles inducing surface plasmon effects, use of different morphologies (1D, 2D, 3D) and assembly of semiconductors Here, amongst these different approaches, we will focus on the elaboration of Au/g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> photocatalysts, in order to optimize the different functions of the composite materials: optimization of the synthesis of C<sub>3</sub>N<sub>4</sub> (under different atmospheres) and TiO<sub>2</sub> (influence of the morphology) semiconductors, high quality heterojunction formation, improved Au deposition leading to enhanced electron traps and co-catalyst properties and study of the SPR (Surface Plasmon Resonance) properties induced by Au NPs.



**Figure1:** (a, b and d) TEM micrographs of 0,5 wt.% Au/(TiO<sub>2</sub>-gC<sub>3</sub>N<sub>4</sub>) (95-5) nanostructures. (c) TEM micrographs of bare g-C<sub>3</sub>N<sub>4</sub>. (e) Histogramm showing Au NPs size distribution. (f) TEM micrographs of 0,5 wt.% Au/ TiO<sub>2</sub>-gC<sub>3</sub>N<sub>4</sub> (95-5) nanostructures, magnification of gC<sub>3</sub>N<sub>4</sub> nanosheet.

### Biography

Valérie Keller is a senior scientist at ICPEES in Strasbourg. She received her Ph.D. degree in Chemistry and Catalysis from the University Louis Pasteur of Strasbourg in 1993. In 1996 she returned to Strasbourg and was appointed as researcher in CNRS, where she is now responsible of the Team "Photocatalysis and Photoconversion". Her main research activities concern photocatalysis for environmental, energy and health applications, and the synthesis and characterization of nanomaterials for photoconversion purposes. She is the author of over 100 publications in peer-reviewed journals and more than 85 oral communications in international conferences and symposium. She is also the author of 15 patents. In 2013 she was awarded the 1st Price of the Strategic Reflection (awarded by the French prime Minister).

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## On unified approach in description of crystalline structures in discrete space

**V. Ya. Shevchenko**

Russian Academy of Sciences, Russia

The geometric crystallography offers two ways of looking at the natural dividing of structures into a large number of unit cells. Usually, the crystal is viewed as consisting of "elementary cells", which are repeated by translation of the lattice. An alternative system also divides the crystal in the identical space-filling polyhedra (including different forms), but they do not necessarily represent the translationally-equivalent figures. These areas are called "areas for interaction", "basic configurations". Such regions may be defined in the n-dimensional space. The concept of homogeneous space can be formulated in two cases: continuous infinite space and infinite discrete space. Traditional crystallography is based on the use of X-ray diffraction, which underlines periodicity, but electron microscopy gives a more general form of the order. In these cases we have images in a geometric cross-sections or projections for analyze. We consider the sections and projections as two-dimensional images therefore relevant Penrose's patterns. Two-dimensional Penrose's patterns can be prepared by projection of five-dimensional hyper cubic lattice in the corresponding direction, and three-dimensional patterns can be prepared from a 6-dimensional hypercube lattice. Consequently, the real discrete space has a dimension in which the cross section and the projection are equivalent because projection in one space (real/converted) corresponds to a section in another one (the transformed/real). This explains an existence of large number of "exceptions" from the "classic" spatial concepts of crystallography, including quasicrystals. The investigation of features of nanostate allowed concluding about its structural many fold. This property determines the local character of formation of nanoparticle, and supports the concept of "building blocks" - the fundamental configurations and, therefore, necessity of use of the space of the high dimensions for the description of various nanoparticles. We can now indicate the main problem for the chemistry of the XXI century – how a substance is produced? The place where it is formed - the nanoworld.

### Biography

Dr. Vladimir Shevchenko was born on 1947, Smela of the Cherkasy region. In 1963 he graduated from the Physics Department of the Moscow State University. M.V. Lomonosov Moscow State University. In 1977 he defended his doctoral dissertation. Since 1998, he is director of the Institute of Silicate Chemistry named after I. Grebenshchikov of the Russian Academy of Sciences. In 1970s, he analyzed the homological series of inorganic substances and discovered the laws of the "dielectric-metal" transitions (USSR Discovery No. 196). He is headed by the Scientific Council of the Russian Academy of Sciences on ceramic and other non-metallic materials of the Russian Academy of Sciences.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Engineering columnar crystals: A novel, template-based method of sequential deposition

**Ho-Kei Chan**

Harbin Institute of Technology, China

Identical hard spheres inside an infinitely long cylinder exhibit a rich variety of densest columnar phases, where many of them are helical. These phases exhibit spatial periodicity, and for this reason such periodic structures are referred to as columnar crystals. The densest structures of such confined systems, and also the corresponding packing fraction and chirality, are independent of length scales, and they depend solely on the dimensionless diameter-ratio  $D$  between the cylinder and the spheres. Like the face-centred cubic (fcc) and hexagonal close-packed (hcp) densest structures of hard spheres, such columnar crystals can also serve as models for structures of matter, where notable examples include the quasi-one-dimensional systems of nanotube-confined fullerenes and colloidal crystal wires. It is therefore believed that a detailed study of this problem of sphere packing would lead to new insights into structures of matter and new inspirations for the design and fabrication of low-dimensional materials. In this talk, I will give an introduction to such densest columnar structures of hard spheres as predicted by computer simulations [Mughal A., Chan H.-K. and Weaire D. (2011) *Physical Review Letters* 106: 115704] for a diameter ratio up to  $D = 2.7013$ , and will present a template-based method of sequential deposition [Chan H.-K. (2011) *Physical Review E* 84: 050302(R)] that can be used for the construction of such structures. As structures constructed via this method of sequential deposition depend sensitively on the configuration of the underlying template, some novel columnar structures that exhibit unexpected ordering, for example a hybrid structure [Chan H.-K. (2013) *Philosophical Magazine* 93, 4057] of the single and double helices, have also been discovered from this method, and they will be covered in this talk as well.



### Biography

Ho-Kei Chan is an Associate Professor

at the Hong Kong Polytechnic University. Chan moved to the University of Manchester for a PhD in physics. This was followed by post-doctoral research in the Hong Kong Baptist University, Trinity College Dublin, and then the University of Nottingham. Chan has published a variety of scientific articles in the fields of statistical, nonlinear, and soft matter physics, most notably his work on a template-based method of sequential deposition for generating a wide range of densest columnar packings of spheres.

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# ADVANCED MATERIALS & PROCESSING

September 07-08, 2017 | Edinburgh, Scotland

## Microstructure development affected by electrode geometry during resistance spot welding

Peng-Sheng Wei

National Sun Yat-Sen University, Taiwan

Resistance spot welding is an important technique often used in joining thin workpieces in different manufacturing, aerospace, aeronautics and automobile industries. This presentation theoretically and quantitatively investigates and interprets processes by realistically accounting for transient magneto-fluid mechanics, heat and species transport, and temperature-dependent bulk resistance in workpiece, and film and constriction resistances at contact interfaces. Since temperature gradient and solidification rate are found, the computed morphological parameter, namely, the ratio between temperature gradient and solidification rate, shows that electrode geometry can be designed to control microstructures of the weld nugget. Figures 1(a) and (b) show that solidification rate decreases whereas heat flux increases as electrode face radius decrease, respectively. A decrease in electrode face radius therefore increases the morphology parameter, leading to columnar dendrites, whereas cooling rates can be decreased or increased.

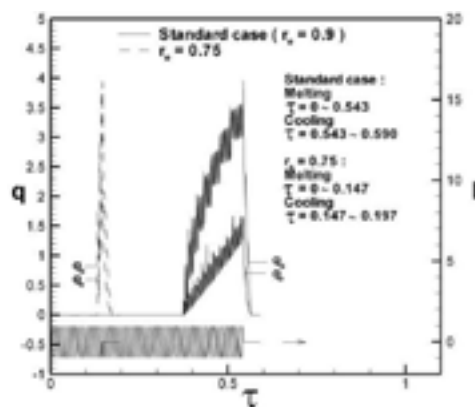


Fig.1 (a) Growth and recession rates of nugget, and (b) heat flux or temperature gradient in radial and axial directions for different electrode face radii.

### Biography

Dr. Peng-Sheng Wei received Ph.D. in Mechanical Engineering Department at University of California, Davis, in 1984. He has been a professor in the Department of Mechanical and Electro-Mechanical Engineering of National Sun Yat-Sen University, Kaohsiung, Taiwan, since 1989. Dr. Wei has contributed to advancing the understanding of and to the applications of electron and laser beam, plasma, and resistance welding through theoretical analyses coupled with verification experiments. Investigations also include studies of their thermal and fluid flow processes, and formations of the defects such as humping, rippling, spiking and porosity. Dr. Wei has published more than 80 journal papers, given keynote or invited speeches in international conferences more than 90 times. He is a Fellow of AWS (2007), and a Fellow of ASME (2000). He also received the Outstanding Research Achievement Awards from both the National Science Council (2004), and NSYSU (1991, 2001, 2004), the Outstanding Scholar Research Project Winner Award from National Science Council (2008), the Adams Memorial Membership Award from AWS (2008), the Warren F. Savage Memorial Award from AWS (2012), and the William Irgang Memorial Award from AWS (2014). He has been the Xi-Wan Chair Professor of NSYSU since 2009, and Invited Distinguished Professor in the Beijing University of Technology, China, during 2015-2017.

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### Notes: