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PROCEEDINGS OF

2ND ADVANCED MATERIALS SCIENCE WORLD CONGRESS 2021

JUNE 14-15 2021 BERLIN, GERMANY

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ADV. MATERIALS SCIENCE 2021

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A CONFLUENCE OF ERUDITE AND KNOWLEDGE-SEEKER

PROGRAM-AT-A-GLANCE

ADV. MATERIALS SCIENCE 2021

DAY 1

MONDAY, JUNE 14, 2021

Scientific Program

BST – British Summer Time

07:45-08:00	**Opening Ceremony**

Keynote Session

08:00-08:25	**Title: Multiscale approaches to monitor the long-term life fate and bio-processing of anticancer heat-mediating nanoparticles and their optimization** **Alberto Curcio,** University Paris Diderot, France
08:25-08:50	**Title: Formation of surface self-assembled organosilicon nanolayers on carbon steel and its effect on electrochemical and corrosion behavior of the metal** **Maxim A. Petrunin,** Russian Academy of Sciences, Russian Federation
08:50-09:15	**Title: Plasma treatment of polyolefin powder – Process and application** **Petr Špatenka,** Czech Technical University, Czech Republic

Sessions: Polymer Science and Technology | Materials Science and Engineering | Materials Characterization, Theory and Modeling | Metals and Alloys | Advanced Materials and Nanotechnology | Nanomaterials and Nanotechnology | Metallurgical and Materials Engineering | Semiconductors

09:15-09:35	**Title: Development of compact solar-pumped lasers** **Tomoyoshi Motohiro,** Nagoya University, Japan
09:35-09:55	**Title: Dynamics of lithium around electrode/solidelectrolyte interface in all-solid-state batteriesunder charging and discharging by ion beam analysis** **Bun Tsuchiya,** Meijo University, Japan
09:55-10:10	**Title: Novel fuel cell using ion channel membrane and its proton conductivity** **Tomoki Furuseki,** Setsunan University, Japan
10:10-10:30	**Title: Automotive CFRP application with structural adhesives** **Hyun-Joong Kim,** Seoul National University, South Korea
10:30-10:50	**Title: Tailoring ordering-disorderingtransition in high-entropy alloy** **Jae Bok Seol,** Gyeongsang National University, South Korea

Refreshment Break 10:50-11:05

11:05-11:25	**Title: Photocatalytic activity of graphitic carbon nitride with tunable morphology and bandgap** **Jinshu Wang,** Beijing University of Technology, China
11:25-11:45	**Title: DFT study on carbon-based 2D materials: Geometric structures, electronic, and magnetic properties** **Ngoc ThanhThuyTran,** National Cheng Kung University, Taiwan
11:45-12:00	**Title: Growth of high-quality GaN by molecular beam epitaxy for the application in high-power and high-frequency electronics** **Thi-Thu Mai,** National Yang Ming Chiao Tung University, Taiwan
12:00-12:20	**Title: Functionalized hyaluronic acids for single-pot self- assembled nanogels as novel delivery platform to improve pharmaceutical bioavailability** **Jittima Amie Luckanagul,** Chulalongkorn University, Thailand
12:20-12:40	**Title: Formation of the structure and properties of chromium-Nickel steel during plasma electrolytic hardening** **Bauyrzhan Korabayevich Rakhadilov,** Sarsen Amanzholov East Kazakhstan University, Kazakhstan
12:40-12:55	**Title: Improving the reliability design of mechanical systems such as refrigerator** **Seongwoo Woo,** Addis Ababa Science & Technology University, Ethiopia
12:55-13:15	**Title: Crystallographic basis of shape reversibility in shape memory alloys** **Osman Adiguzel,** Firat University, Turkey

Lunch Break 13:15-13:45

13:45-14:05	**Title: Long-acting injectable antipsychotics: Contemporary formulations andsynthesis methods** **Burcu Ertug,** Nişantaşı University, Turkey
14:05-14:25	**Title: From metallic to semiconductor conversion of single –walled carbon nanotubes by chlorination** **Mourad Berd,** Université de Bejaia, Algeria
14:25-14:45	**Title: Hybrid Drug Nanoforms with Metal Nanoparticles in the Controlled Antibiotic Drug Delivery** **Tatyana I. Shabatina,** Moscow State University, Russian Federation
14:45-15:00	**Title: The effect of functional additives on the structure and properties of PHB-based nanofibers** **Tyubaeva Polina,** Plekhanov Russian University of Economics institute, Russian Federation

15:00-15:20	**Title: Biodegradable polymers based on polyolefins and elastomers** **Ivetta Varyan,** Russian Academy of Sciences, Russian Federation
15:20-15:40	**Title: Modern elastomers using anisotropic carbon based fillers** **Ulrich Giese,** German Institute of Rubber Technology, Germany
15:40-16:00	**Title: Modeling and simulation of micro-structural material properties and reactive injection mouldingin polyurethane foams** **Konrad Steiner,** Fraunhofer Institute for Applied Mathematics ITWM, Germany
Refreshment Break 16:00-16:15	
16:15-16:35	**Title: How to test the arrhenius validity of elastomers during ageing** **Maha Zaghdoudi,** Bundesanstalt für Materialforschung und -prüfung (BAM), Germany
16:35-16:55	**Title: Insights into the bead fusion mechanism of expanded polybutylene terephthalate (E-PBT)** **Holger Ruckdaeschel,** University of Bayreuth, Germany
16:55-17:10	**Title: Time optimization of seed-mediated gold nanotriangle synthesis based on kinetic studies** **Ekaterina Podlesnaia,** Leibniz Institute of Photonic Technology(IPHT), Germany
17:10-17:30	**Title: Strengthening aluminium alloys under as-cast condition for high pressure die casting** **Shouxun Ji,** Brunel University, United Kingdom
17:30-17:50	**Title: Emerging non-volatile electronic memory devices from polymers to transition metal oxides** **Iulia Salaoru,** De Montfort University, United Kingdom
17:50-18:05	**Title: A hierarchical bayesian calibration of data-driven models for composite laminate consolidation** **Nikolaos Papadimas,** University of Exeter, United Kingdom
End of Day 1	

DAY 2

TUESDAY, JUNE 15, 2021

Scientific Program

BST – British Summer Time

Keynote Session

07:45-08:00	**Opening Ceremony**
08:00-08:25	**Title: RE-based magnetic materials for e-mobility** **Spomenka Kobe,** Jožef Stefan Institute, Slovenia
08:25-08:50	**Title: Electrochemical corrosion resistance of polyetheretherketone-based coatings electrophoretically deposited on the Ti-6Al-4V alloy** **Alicja Lukaszczyk,** AGH University of Science and Technology, Poland
08:50-09:15	**Title: Influence of coupling two additive-manufacturing technologies on the microstructure of nickel alloys** **Matjaz Godec,** Institute of Metals and Technology, Slovenia

Sessions: Composite Materials | Polymer Science and Technology | Materials Science and Engineering | Materials Synthesis and Processing | Metals and Alloys | Metallurgical and Materials Engineering | Carbon and 2D Materials | Surface Science and Engineering | Nanomaterials and Nanotechnology | Metals and Alloys

09:15-09:35	**Title: Grain-boundary segregation of boron in high-strength steel: Characterization and modelling** **Philippe Maugis,** Aix Marseille University, France
09:35-09:55	**Title: Repair of components using additive manufacturing technologies** **Wilfried Pacquentin,** Université Paris-Saclay, France
09:55-10:15	**Title: A greener approach to the solution combustion synthesis of mixed oxides: Role of the chemical precursors** **Francesca Deganello,** Italian National Research Council, Italy
10:15-10:35	**Title: On the interaction of carbon nanotubes with photosynthetic assembles** **Maya Dimova Lambreva,** National Research Council(CNR), Italy
10:35-10:55	**Title: Ni-based catalysts for CO_2 conversion into CH_4: Advances in catalysts design and promotion effects** **Leonarda Francesca Liotta,** National Research Council(CNR), Italy

10:55-11:15	**Title: Direct laser patterning of photoluminescent semicondutor quantum dots in polymeric films** **Francesco Antolini,** ENEA Frascati Research Center, Italy
Refreshment Break 11:15-11:30	
11:30-11:50	**Title: Microneedles fabrication technology for sensing and therapeutic applications** **Principia Dardano,** Institute of Applied Science and Intelligent Systems, Italy
11:50-12:10	**Title: High performance Lithium Silicide electrode enable by molecular layer deposition** **Zahilia Cabán Huertas,** Aalto University, Finland
12:10-12:30	**Title: An efficient four-variable I-L nonlocal dynamic model of unsymmetrical plane sandwich structure with laminated facings – Acoustic application** **Stanisław Karczmarzyk,** Warsaw University of Technology, Poland
12:30-12:50	**Title: Microstructure dependent corrosion of Mg-Li alloys** **Anna Dobkowska,** Warsaw University of Technology, Poland
12:50-13:10	**Title: Monitoring the effect of amino acid on the corrosion process of metal based on comprehensive micro- and nanospectroscopy investigations** **Dominika Swiech,** AGH University of Science and Technology, Poland
Lunch Break 13:10-13:40	
13:40-13:55	**Title: W-Zr-B coatings deposited by RF Magnetron – PLD hybrid method** **Rafał Psiuk,** Polish Academy of Sciences, Poland
13:55-14:10	**Title: Photoluminescence of carbon nanoparticles synthesized by laser ablation in water and aqueous solutions of amine-based reagents** **Agata Kaczmarek,** Polish Academy of Sciences, Poland
14:10-14:25	**Title: Analysing the impact of hydrophobic coatings on the reduction in soil accumulation on transparent surfaces intended for PV application** **Małgorzata Rudnicka,** Gdańsk University of Technology, Poland
14:25-14:40	**Title: The effect of plasma treatment of polyethylene powder on the mechanical properties of composites prepared by rotational molding** **Zoya Ghanem,** Czech Technical University, Czech Republic
14:40-14:55	**Title: Ensuring electrical conductivity of polymer-based component** **Jakub Antoň,** Czech Technical University, Czech Republic

14:55-15:15	**Title: Solid materials as green catalysts for bioenergy processes: A review as a sustainable perspective** **Jaime Filipe Borges Puna,** Instituto Superior de Engenharia de Lisboa, Portugal
15:15-15:35	**Title: Functionally-graded materials and complex alloy systems through wire-arc additive manufacturing** **Thomas Klein,** Austrian Institute of Technology, Austria
15:35-15:55	**Title: Electron concept for hydrogen brittleness of metals** **Valentin Gavrljuk,** Kyiv Academic University, Ukraine
15:55-16:15	**Title: Preparation, investigation and widespread utilization of bacterial cellulose-ZnO-MWCNT hybrid membranes** **Zoltan Nemeth,** University of Miskolc, Hungary
Refreshment Break 16:15-16:30	
16:30-16:50	**Title: Synthesis of $ZnTiO_3/TiO_2$ nanocomposite supporting in Ecuadorian clays for the adsorption and photocatalytic degradation of methylene blue** **Ximena Jaramillo-Fierro,** Universidad Técnica Particular de Loja, Ecuador
16:50-17:10	**Title: Microstructure conditioning in an advanced boron-containing complex phase steel heat treated within the Q&P process concept** **Antonio Enrique Salas Reyes,** National Autonomous University of Mexico(UNAM), Mexico
17:10-17:30	**Title: Effect of cooling rate and alloying elements on Al-Si-Fe alloys** **Ignacio Alejandro Figueroa,** National Autonomous University of Mexico(UNAM), Mexico
17:30-17:50	**Title: Increment of CO_2 adsorption capacity of nanostructured wool activated carbon fibers by nitrification** **Alejandro Amaya,** Universidad de la República, Uruguay
17:50-18:05	**Title: Direct synthesis and pH adjustment approaches to incorporate zirconium species in SBA-15 mesoporous silica** **Julio Colmenares-Zerpa,** University of Concepción, Chile
18:05-18:15	**Title: Extraction chromatography materials prepared with MIBK on amberlite®XAD4 and PTFE** **Fabiola Monroy-Guzmán,** The National Institute for Nuclear Research (ININ), Mexico
End of Day 2	
Closing Remarks	

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2ND ADVANCED MATERIALS SCIENCE WORLD CONGRESS 2021

June 14-15
2021

Keynote Presentations

Day 1

PEERS ALLEY MEDIA

Theme: Navigating the future research directions in the field of Materials Science and Engineering

2nd Advanced
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BIOGRAPHY

After a master in Medical Biotechnology, he obtained his PhD in 2013 at Italian Institute of Technology of Genoa where he developed multifunctional stimuli-responsive nanomaterials for drug/gene delivery, MRI imaging and magnetic hyperthermia therapy, alongside carrying out biomolecular functionalization, gene expression and nanotoxicology studies. Since 2016 he joined the Prof. Claire Wilhelm's biophysics group as postdoc at Paris Diderot University. His research is focused on the study of magnetic, plasmonic and photodynamic cancer nano therapy, as well as the characterization of nanoparticles biodegradation and long term fate in 3Dstem tissue. Recently he developed different murine cancer models for magnetic targeting and bio distribution.

A. Curcio

University Paris Diderot, France

Multiscale approaches to monitor the long-term life fate and bio-processing of anticancer heat-mediating nanoparticles and their optimization

In recent years, increasing interest has risen toward innovative nanomaterials engineering and tailor-made applications of nanomedicine compositions. As a result, the follow-up of potential degradation of these complex nanohybrids has become central for their future medical use.

We investigated the fate of several anticancer heat-mediating nanoparticles upon interaction with different biological model systems using thermometric and magnetic measurements, as well as methods of structural analysis (XANES/EXAFS spectroscopy and HR-TEM), as direct and quantitative assessment of the bio-transformations in the tissues. Furthermore, nanotoxicology and gene expression studies addressed the impact of the nanoparticles on the cell metabolism, the cell viability or their differentiation.

All nanostructures analyzed underwent profound biotransformation that triggered an adaptation of the cellular metabolism to the released metals. Besides, a massive intracellular remodeling of the nanoparticles could originate newly formed biogenic nanostructures and, depending from their composition, can preserve or not the therapeutic efficacy.

Both nanomaterials' intracellular performances and their biocompatibility including their ultimate fate inside the human body need to be extensively monitored in long-term analysis in order to ensure their applicability into the clinic. Furthermore, the therapeutic potential of heat-generating nanoparticles is limited to a specific temporal period that is often overlooked but is central for their medical applications.

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BIOGRAPHY

Maxim A. Petrunin is graduated from Lomonosov Moscow State University Chemical Department, Speciality"Chemistry (chemist) in 1985. He completed PhD at the Institute of Physical Chemistry of the Russian Academy of Sciences, Speciality "Chemical resistance of materials and corrosion protection in 1991. Present working as a Head of scientific sector (working group) of underground corrosion nand electrochemical protect. Specialist in Corrosion Monitoring, Stress corrosion Cracking, underground corrosion. Scientific researcher in the field of physical chemistry, electrochemistry, corrosion sciences, formation of functional nanocoatings on metal surfaces.

M.A.Petrunin

Russian Academy of Sciences, Russian Federation

Formation of surface self-assembled organosilicon nanolayers on carbon steel and its effect on electrochemical and corrosion behavior of the metal

With the using Fourier transformed infrared (FT-IR) spectroscopy, scanning electron spectroscopy(SEM) and energy dispersive x-ray spectroscopy(EDX), the adsorption of vinyltrimethoxysilane on the surface of carbon steel from an aqueous solution and surface self-assembled organosilicon nanolayers formation have been studied. The mechanism of formation of the surface self-assembled nanolayer is proposed. It has been shown that during adsorption organosilanes interact with hydroxil radicals of a metal surface with Fe-O-Si bonds formation.

The effect of organosilicon nanolayers on the electrochemical behavior of carbon steel was studied by obtaining anodic polarization curves. It is shown that the presence on the surface of vinyl and diamine-containing siloxane nanolayers on the surface leads to a significant reduction in the critical passivation current of steel, i.e. surface organosilicon nanolayers contribute topassivation of steel.

In addition, it have been found that in the presence of organosilicon nanolayers on a metal surface causes the shift of critical potential of pitting formation of steel to the region of positive values, which indicates the inhibition of localized anodic dissolution of the metal. Accelerated corrosion tests of steel samples in the climatic chamber were carried out and the corrosion inhibiting effect of vinyl-containing surface nanolayers was shown.

It have been established that vinyl-containing soiloxane surface self-assembled nanolayer is resistant to anodic polarization action, which usually contributesunifiorm and localized dissoltution of metals. As have been shown by FT-IR spectroscopy, the surface nanolayer is presented on a metal surface after anodic polarization. The results obtained indicateon the stability of siloxane nanolayers to water and corrosion-active components of an electrolyte action and to change of surface morphology due to dissolution of surface metal atoms with the release of metal ions into solution.

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BIOGRAPHY

Petr Špatenka received the M.Sc. degree in physics and mathematics and the Ph.D. degree in plasma physics from the Faculty of Mathematics and Physics, the Charles University in Prague in 1978 and 1986, respectively. He was employed at the University of South Bohemia and the Technical University in Liberecs, Cyech Republic and at the University of Tübingen, Germany. Now he is the head of Department of Materials Engineering at the Czech Technical University in Prague. His research interests include plasma diagnostics, plasma chemical processes and their application for surface treatment, plasma treatment for biological applications and deposition of functional coatings. He is the founder of the PlasmaTech Ltd. and the president of the Surface Treat Inc. companies.

P. Špatenka

Czech Technical University, Czech Republic
Surface Treat Inc., Czech Republic

Plasma treatment of polyolefin powder – Process and application

Polyethylene powder (PE) of average particle diameter of 160 μm was activated in a laboratory plasma reactor made from aluminum of volume 64 dm 3 at the pressure 100 Pa. Air and oxygen plasma were sustained with a microwave discharge powered by a pulsed magnetron source of power 1 kW. The evolution of powder wettability versus treatment time was measured using the Washburne method. Presence of polar groups on plasma treated powder was determined by X-ray Photoelectron Spectroscopy (XPS).

Role of plasma penetration between particles was investigated. It was proved that certain degree of hydrophylization occurred up to 10 mm down under the upper layer of the powder. This penetration significantly contributes to the efficiency of powder treatment in large-scale applications. The penetration decreases with lowering the particles diameter and disappears for particles lower than some 20 μm.

The plasma treated PE evidence adhesion enhancement to various materials. Plasma treated PE reaches joint strength with chrome and steel of 7.2 and 10.3 MPA respectively. The adhesion also resulted in improvement of mechanical properties of composite materials with PE matrix with glass or natural fibers. The tensile strength of samples prepared from plasma treated PE increased up to 74% in comparison with samples made from non-treated PE.

Based on the laboratory experiments an industrial-scale set-up has been constructed. Some examples form industrial application of plasma treated powder will be presented.

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Scientific Abstracts

Day 1

PEERS ALLEY MEDIA

Theme: Navigating the future research directions in the field of Materials Science and Engineering

2nd Advanced MATERIALS SCIENCE WORLD CONGRESS 2021

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Development of compact solar-pumped lasers

T. Motohiro[1], H. Ito[1] and K. Hasegawa[2]

[1]Nagoya University, Japan

[2]Graduate School for the Creation of New Photonic Industries, Japan

We have developed a compact solar-pumped laser (μSPL) employing an off-axis parabolic mirror with an aperture of 76.2mm diameter and an Cr doped Nd (0.1 at %): YAG transparent ceramic rod of φ1 mm x 10 mm as a laser medium (LM). Here, the stimulated emission takes place by the transition of Nd^{3+} in YAG from its excited state to lower energy states. Cr is doped to absorb the sunlight in broad wavelength ranges and to transfer the absorbed solar energy to Nd^{3+} because Nd^{3+} absorbs the sunlight only in the limited narrow wavelength ranges. The laser oscillation wavelength of 1.06 μm, just below the optical absorption edge of Si solar cells, is suitable for photoelectric conversion with minimal thermal loss after optical wireless (laser) power transmission to distant places. The small LM and solar concentrator realize more stable oscillation by rapid natural/air convection cooling and increased mechanical stability during wind exposure in contrast to the conventional large SPLs employing typically a 2 m size solar concentrator. Outdoor operation tracking the sun yielded continuous oscillation exceeding 6.5 h, improving upon the previously reported 11 min. This showed applicability of SPLs to whole day operation and terrestrial solar energy utilization. Here, the SPL output increased more than eightfold between LMs with Cr contents of 0.0 and 0.4 at%, and then decreased at 0.7 at% and further at 1.0 at%, where the round-trip loss due to scattering by Cr dopants became significant. Energy transfer efficiencies from Cr^{3+} to Nd^{3+} were assessed to be lower than 50%. This can be attributed to the fact that the energy transfer from excited Cr^{3+} to unexcited Nd^{3+} became difficult because Nd^{3+} had been already excited directly by the sunlight. Although Cr doped Nd: YAGs are renowned LMs, development of more efficient LMs for SPL sis eagerly awaited.

Biography

Tomoyoshi Motohiro has been a researcher of applied physics working on superconducting magnetic energy storage, solar-pumped lasers, solar-cells, optical recording and transient analysis of surface catalytic reactions, thin film retardation plates and thin film processes. 2019-Present Visiting Prof., Nagoya Univ., Japan. 2012-2019 Prof., Graduate School of Engineering, Nagoya Univ. Japan.2007-2013 Senior Fellow, Toyota Central R&D Labs., Inc., Japan. 2006-2017 Visiting Prof., Toyota Technological Institute., Japan. 1978-2006 Researcher and Research Manager, Toyota Central R&D Labs.,Inc., Japan. D.Eng. The University of Tokyo Graduate School of Eng., 1986. M.Eng. The University of Tokyo Graduate School of Eng., 1978. B. Eng. The University of Tokyo, 1976.

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Theme: Navigating the future research directions in the field of Materials Science and Engineering

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Dynamics of lithium around electrode/ solid electrolyte interface in all-solid-state batteries under charging and discharging by ion beam analysis

B. Tsuchiya[1] and **K. Morita**[2]

[1]*Meijo University, Japan*

[2]*Nagoya Industrial Science Research Institute, Japan*

Anoxide-based solid-state rechargeable lithium ion (Li^+) batterie is one of the most remarkable next genertion devices. To realize the product, it is essential that we have information on the Li^+ ion transfer resistance at electrode/solid electrolyte interfaces and grain boundaries in the solid-state Li^+ ion batteries. In particule, the Li deficient region formed around the interface during the charging and discharging, which is indicative of space charge layer, locally provides less Li^+ ionconduction and then leads to the interfacial Li^+ ion transfer resistance, since the Li+ionic conductivity in the solid electrolyte significantly depends on the number of Li^+ ion mobile carriers. Thus, the Li distribution around interface in static or operated solid-state Li^+ ion batteries should be clarified well.

In the study, we have *in situ* investigated the static Li distributions around each $LiCoO_2$ positive electrode/$Li_{1+x}Al_xGe_yTi_{2-x-y}P_3O_{12}$–$AlPO_4$(LATP) electrolyte and $LiMn_2O_4$ positive electrode/$Li_{3.3}PO_{3.8}N_{0.2}$(LiPON) electrolyte/Nb_2O_5 negative electrode interface in Au/$LiCoO_2$/LATP/Pt and Ti/$LiMn_2O_4$/LiPON/Nb_2O_5/Ti batteries with charging and discharging by combined ion beam analysis of high-energy elastic recoil detection (ERD) and Rutherford backscattering spectrometry (RBS)techniques using 9.0MeV oxygen ion (O^{4+}) and 5.0MeV heliumion (He^{2+}) probe beams from a tandem accelerator.

The ERD spectra with reliable depth resolution in a few tens of nm scale revealed the that the Li concentration in the positive (negative) electrode uniformly decreased (increased) at several depths with increasing the applied voltages and the Lidepletion region was formed inside the solid electrolyte at the interface with the thickness of approximately 120 ± 30 nm.

Biography

Bun Tsuchiya is a professor at Meijo University. He belongs to Japan.He completed his doctor's degree in materials science from Nagoya University, Nagoya city. He joined the Institute for Materials Research in Tohoku university as assistant professor in April 1998 and the Faculty of Science and Technology in Meijo University as associate professor in April 2010 and as professor in April 2017. He has many international research contributions on the energy materials related to nuclear fusion, fuel cell, and lithium ion battery. His major interest is to investigate the behaviors of some elements with low atomic numbers such as hydrogen, helium, and lithium, and so on in the many different kinds of materials such as metals, semiconductors, and insulators using ion beam analysis. His recent project is to clarify the migration of lithium ions at the interface between the positive- and negative-electrodes and solid-electrolytes in the all-solid-state lithium batteries by charging and discharging using combined elastic recoil detection with Rutherford backscattering spectrometry techniques.

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Novel fuel cell using ion channel membrane and its proton conductivity

T. Furuseki and **Y. Matsuo**
Setsunan University, Japan

Currently, many studies on fuel cells are conducted toward the realization of a hydrogen energy society. Significantly, many investigations concerning fuel cell electrolytes of low cost and high-proton conductivity are carried out. It is also well known that biomaterials are abundant in nature and environmentally friendly materials. In this study, we have fabricated a new fuel cell using ion channel membrane as electrolytes, which are biomaterials with high ionic conductivity, and investigated their electrical properties. The squid axon is used as the ion channel electrolyte. Squid axons have often been used to study ion channels and have suitable properties as electrolytes of fuel cells. The i-V characteristics in the fuel cell using the squid axon electrolyte at 100% relative humidity. The maximum power density of the fuel cell with the ion channel membrane was 0.78 mW/cm^2. Furthermore, we have obtained the result that the power of the fuel cell using the squid axon membrane remarkably decreases by blocking the ion channels using a channel blocker. These results indicate that the fuel cell using the squid axon as the electrolyte operates by the function of the ion channel. In addition, in order to investigate the relationship between proton conductivity and relative humidity, we have carried out the impedance measurement. It was found that the proton conductivity of the squid-axon electrolyte drastically increases at a relative humidity of 85% to 96%. From these results, it is deduced that higher proton conductivity of the squid-axon electrolyte above 96% relative humidity is caused by the activation of ion channels closely related to the fractionalization of water molecule clusters. These results indicate that the fuel cell using the squid-axon membrane becomes the fuel cell using the activation of the ion channel above 96% relative humidity.

Biography

Tomoki Furuseki is a Ph.D. student at Setsunan University majoring in life sciences.

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Automotive CFRP application with structural adhesives

Hyun-Joong Kim
Seoul National University, South Korea

In the automotive manufacture industries weight reduction has become an essential factor due to the national and international regulations for the fuel efficiency. Using carbon fiber reinforced plastic (CFRP) on automotive is one of the reasonable strategies for the regulatory response since not only it can contribute to the light weighting but also it can improve driving performance, assembly time, shock safety and stability. Conventional welding and mechanical joining technologies are inadequate in CFRP application on the vehicle manufacture because of CFRP laminate damaging in a machining process and stress concentration at mechanical joints. The adhesive bonding technologies that can distribute the stress evenly at a face to face joint have been considered as a solution for those problems on CFRP application. However, using CFRP with adhesives for the application is not a simple problem because of the adhesion disturbance factors on CFRP surface and the resin weakness on shock in conventional CFRPs. In the presentation, several types of CFRP manufacturing method and those applications are reviewed for understanding backgrounds. Continuously, some novel surface treatment methods for enhancing adhesion performance and CFRP resin modification for reinforcing shock resistance are suggested, and adhesion performances with surface analysis are reviewed and discussed.

Biography

Hyun-Joong Kim is Professor and Director at Smart Center for Adhesion Research & Development. He completed PhD in Adhesion Science, The University of Tokyo, Japan (March 1995). He completed MS in Coating Science, Seoul National University (February 1989) and BS Forest Products, Seoul National University, Korea (February 1987).

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Theme: Navigating the future research directions in the field of Materials Science and Engineering

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Tailoring ordering-disordering transition in high entropy alloy

J.B. Seol[1], J. Moon[2], J.G. Kim[1], H.K. Sung[1], H.S. Kim[2] and H.J. Bae[1]

[1]Gyeongsang National University, South Korea
[2]POSTECH, South Korea

While X-ray and electron diffraction techniques are typically exploited to identify the existence of short-range order (SRO) in metallic solid solutions, systematical approach to reveal the degree or tendency of SRO is still lacking due to its very tiny length-scale dimension. Further, impact of the SRO tendency on the mechanical properties in metals and alloys still remains a prime challenge in the field of high-entropy alloys with complex chemical flexibility. We report here a strategy that determines the degree or tendency of SRO in a face-centered cubic (FCC) high-entropy alloy (HEA) by monitoring the intensity of diffuse scattering in electron diffraction patterns, by detecting synchrotron X-ray diffuse scattering, and by observing specific heat evolution reaction. When an interstitial $Fe_{40}Mn_{40}Cr_{10}Co_{10}$ (at%) disordering HEA was subjected to tensile loading at 77 K, both the ductility and the ultimate tensile strength of the alloy increased with increasing strain rate, but there was no significant change in yield strength. This phenomenon of neither stress- nor strain-controlled failure is attributed primarily to the advent of deformation-induced SRO domains and their development in disordered structure. The current approach quantitatively demonstrates that tension at high strain rates enhances the intensity of SRO-induced electron scattering as well as an exothermic reaction. Any other TEM laboratory can verify the existence of SRO phenomenon as well as its tendency in other FCC base disordering solid solutions. Further important message in this talk is that disordering-to-ordering transition is common in metallic solid solutions, which are driven by alloy compositions, loading temperatures, and loading rates.

Biography

Jae Bok Seol an Associate Professor at Gyeongsang National University. He belongs to South Korea. He completed his PhD in Department of Materials Science and Engineering, POSTECH. He worked as a Research Professor in National Institute for Nanomaterials Technology (NINT), POSTECH from Apr. 2015 - Mar. 2020. Senior Engineer in Samsung Display R&D center, SAMSUNG (Apr. 2013 - Mar. 2015). Postdoctoral Fellow in Department of Microstructure Physics and Alloy Design, Max-Planck-Institut für Eisenforschung(Sep. 2011 - Mar. 2013). His major research interests are "Thermo-Mechanical Process Design" "Microstructure Characterization".

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Photocatalytic activity of graphitic carbon nitride with tunable morphology and bandgap

Jinshu Wang
Beijing University of Technology, China

Polymeric carbon nitride (C_3N_4) is an important photocatalyst due to its suitable band edge positions whose energies encompass both potentials of H^+ reduction and H_2O oxidation. However, the efficiency of photocatalysis is still quite low in solar energy converting due to the rapid recombination rate of photoinduced electron-hole pairs. Herein, we constructed heterojunction on the surface of C_3N_4 materials and studied the photocatalytic property.

We presented a facile molten salt-assisted route to prepare red-color and water soluble g-C_3N_4 nanosheets with whole red-shift absorption and narrowed bandgap of 1.9 eV for sensitization of TiO_2. Both experimental findings and theoretical calculations revealed that alkali heteroatoms modification led to the surface structure and electronic structure changes. The red-color carbon nitride showed enhanced visible-light absorption and charge transfer efficiency compared with general yellow-color carbon nitride. By hybridization with TiO_2 photoanode, the modified TiO_2 photoanode generates a photocurrent of approximately 2.33 mA cm^{-1} without any cocatalyst at 1.23 V versus reversible hydrogen electrode under Air Mass 1.5G illumination, which was 2.6 folds higher than that of bare TiO_2 photo anode. Recently, we developed a new post-redox strategy to achieve reduced few-atom-thick C_3N_4(FAT-C_3N_4)with controllable C-reduction and electron rich π-conjugated structure, which is different from existing exfoliation methods. Few-atom-thick C_3N_4 and the as-prepared carbon-reduced few-atom-thick C_3N_4 (CRed-FAT-C_3N_4) were obtained. The CRed-FAT-C_3N_4 possesses few number of periodic stacking layers, which suggests the transformation from thick C_3N_4 aggregates into apparent porous nanosheets, and the thickness of CRed-FAT-C_3N_4 is about 1.0 nm, corresponds to three and four single layers. CRed-FAT-C_3N_4 exhibits the supreme photocatalytic hydrogen evolution efficiency of 12.31 mmol h^{-1} g^{-1} (calculated from the first 5 h-cycle), which is about 17-fold enhancement of pristine C_3N_4 and much higher than that of FAT-C_3N_4 and CRed-C_3N_4.

Biography

Jinshu Wang Professor of Faculty of Materials & Manufacturing, Beijing University of Technology. She received her Ph. D degree majoring in Materials Science from Beijing University of Technology. From 2002 to 2004, she has been worked in Tohoku University, Japan, as a post-doctor. She was awarded the Distinguished Professor of Chang Jiang Scholars Program by the Ministry of Education, China in 2015. She received National Science Fund for Distinguished Young Scholars in 2012, and China Youth Science and Technology Award authorized by the China Association for Science and Technology in 2011. Her research interests encompass electron emission materials, photocatalysts for hydrogen production and pollution control.

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DFT study on carbon-based 2D materials: Geometric structures, electronic and magnetic properties

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National Cheng Kung University, Taiwan

Due to the remarkable properties, graphene-based system is considered as one of the promising materials for electronic devices. This study presents a systematic review on the geometric, electronic and magnetic properties adatom adsorption on graphene by means of the density functional theory (DFT) calculations. The geometric and electronic properties are greatly diversified by the the distinct adatom adsorptions and concentrations. The electronic structures consist of the carbon-, adatom- and (carbon, adatom)-dominated energy bands. The semi-metallic or semiconducting behaviors of graphene-related systems are dramatically changed by the multi- or single-orbital chemical bondings between carbons and adatoms. Apart from graphene, another 2D carbon-based materials, FeC, have attracted a great interest of the scientific community due to their unique behaviors including the magnetic and catalytic ones which may lead to the potential applications in nanodevices. In this work, the geometric structure, stability, electronic structures and magnetic behaviors of the 2DFeC compounds with square and triangle lattice structure are studied by the DFT calculations. The phonon dispersion calculations and binding energy show that the 2D FeC with puckered triangle lattice structure is the most stable form. Both forms of the 2D FeC compounds are metallic and ferromagnetic materials, however, the mean atomic magnetic moment of Fe in the puckered 2D tr-FeC is significantly smaller than that of the flat 2D t-FeC.This work could serve as a first step towards further investigation into other necessary properties of carbon-based 2D materials for fabrication and potential device applications.

Biography

Ngoc ThanhThuy Tran obtained her Ph.D. in physics in 2017 from the National Cheng Kung University (NCKU), Taiwan. Afterward, she began to work as a postdoctoral researcher and then an assistant researcher at Hierarchical Green-Energy Materials (Hi-GEM) Research Center, NCKU. Her scientific interest is focused on the fundamental properties of 2D materials and rechargeable battery materials by means of the first-principle calculations.

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Growth of high-quality GaN by molecular beam epitaxy for the application in high-power and high-frequency electronics

Thi-Thu Mai, Jin-Ji Dai, Ssu-Kuan Wu, Elica Heredia, Sa-Hoang Huynh and **Wu-Ching Chou**
National Yang Ming Chiao Tung University, Taiwan

High electron mobility transistors (HEMTs) fabricated using AlGaN/GaN heterostructures grown on Si substrate havegained tremendous attention for high-speed and high-power electronic device applications. However, improving the crystal quality of the AlGaN/GaN hetero structure in order to achieve better device performance remains challenging. Recently, the growth technique of SiNx nano-mask grown via metal-organic chemical vapor deposition (MOCVD) was applied to improve the quality of the AlGaN/GaN heterostructure. A reduction in edge-type threading dislocation density was observed, which results in improving2DEG electronic properties. However, the organic precursors involved in the MOCVD technique inadvertently introduce undesirable impurities that could degrade the crystal quality. In addition, the high-temperature growth of MOCVD and thicker buffer layer could induce cracks and wafer bowing. This work evidences that theplasma-assisted molecular beam epitaxy (PAMBE) technique can efficiently support the growth of high purity epitaxial film under ultra-high vacuum and lower growth temperature conditions. High-quality GaN grown by PAMBEwith significantly reduced threading dislocation density and defects is confirmed by the X-ray and photoluminescence (PL) measurements. The enormously reduced yellow (YL) and blue luminescence (BL) intensity implies a huge reduction in point defects and impurities compared with the GaN/Si template, improved compressive stress in GaN layer by PAMBE is observed by the Raman scattering. Atomic force microscope (AFM) images also reveal smooth morphology with a root mean square roughness of less than 0.5 nm. Reduced pit density and dislocation are investigated by the scanning electron microscope (SEM) images and X-ray measurement, respectively. The above results are further verified by the cathodoluminescence measurements. In summary, high-quality GaN was grown by PAMBE for the application in high-speed and high-power electronic HEMT devices.

Biography

Thi Thu Mai is a Doctoral Student at the Department of Electrophysics, National Yang-Ming Chiao Tung University (NYCU) in Taiwan. She completed her masters at the Department of Condensed Matter Physics, Ha Noi National University of Educations, Ha Noi, VietNam. She has been working on fabrication of III-V semiconductors for high-electron mobility transistors, focusing primarily on PAMBE and MOCVD techniques. Her works involve doping materials like carbon, iron, magnesium to achieve high-resistivity buffer layers for high-power and high-frequency electronic applications. In order to improve device performance and investigate through techniques such as Cathodoluminescence, high resolution X-ray diffraction, raman spectroscopy, photoluminescence, atomic force microscopy, and scanning electron microscope.

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Functionalized hyaluronic acids for single-pot self- assembled nanogels as novel delivery platform to improve pharmaceutical bioavailability

J.A. Luckanagul and **T. Kaewruethai**
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Objective and Scope: In recent years, many studies indicated that curcumin possesses pharmacological effects in cellular studies such as anti-inflammatory, anti-bacterial, anti- cancer including wound healing effect. However, poor solubility and stability issue of curcumin brought about the huge challenge for bioavailability of the drug to its targets.

According to the colloidal stability of nanogel, the delivery system was chosen to overcome the difficulties. Functionalized hyaluronic acids (f-HAs) are modified polymers, which were developed as materials forming nanogels for the best outcome in delivering the powerful cargos.

Methods: The polymers were characterized by NMR for the successful polymer grafting and the interaction between drug and materials was confirmed by FTIR. Besides, f-HA nanogels were assessed for their biocompatibility using metabolic-rate assay with L929 cells. The nanogel-assist internalization of drug into cells was also performed.

Results: Functionalized hyaluronic acids nanogel presented the distinct drug encapsulation efficiency at 87.84% and drug release under 37°C indicated drug delivery property of this system. The results showed that 0.5%w/v of polymer in water is biocompatible to fibroblast cell line (L929). Moreover, the nanogels loaded with curcumin further promoted cell growth compared with non-treated cells showing the potential wound healing activity. The nanogel could also promote drug uptakes.

Conclusion: The design of self-assembled nanogels based on single-pot process was achieved with the f-HAs. The potential benefit of the system towards industrialization of polymer nanotechnology has been improved. With further animal studies and clinical trials, the materials could be the future of drug delivery system to be used in biomedicines.

Biography

Since 2016, Assistant Professor Jittima Amie Luckanagul is a faculty member at Pharmaceutical Sciences, Chulalongkorn University, where she received her Bachelor of pharmacy in 2008. In 2009, she started her graduate research at the University of South Carolina in Biochemistry and received her Ph.D. in the class of 2014. Her background in pharmaceutics, physical pharmacy, biomaterials, and nanotechnology spear her research direction into designing novel delivery systems for biotherapeutics and testing platform for drug and health products. Apart from her academic specialization, she has extensive experience working with nanomaterials for biomedical uses and system/material analyses, through a spin-off company in the U.S. and Thailand. She is a full-time lecturer for 12 under- graduate classes and 5 graduate classes. She focuses on research work from basic sciences to the applications. She has her mission on pushing research to the market and be a part to drive value-based economy by innovation and creativity.

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Formation of the structure and properties of Chromium-Nickel steel during plasma electrolytic hardening

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This work is devoted to research the effect of plasma electric hardening (PEH) on changing in the phase-structural and tribological properties of 0.34C-1Cr-1Ni-1Mo-Fe steel, which used for the manufacture of heavily loaded gears. PEH of steel samples was performed on an installation that consists of a power source, an electrolyte-plasma material processing chamber, and a personal computer. The process of electrolytic-plasma hardening of steel samples 0.34C-1Cr-1Ni-1Mo-Fe was performed in electrolyte containing an aqueous solution of 20 % calcined soda (Na_2CO_3) and 10 % carbamide ($(NH_2)_2CO$). Morphological and elemental analysis of the samples was performed using a JSM-6390LV scanning electron microscope. The phase composition of the samples was researched by X-ray diffraction analysis using X'PertPRO diffractometers. Research of the morphology of the thin structure was performed on an EM-125 electron microscope at an accelerating voltage of 125 kV. The micro-hardness of steel samples was measured using the Vickers method on the PMT-3 device. For the samples, the nano hardness of the coatings was determined using the Oliver and Farr nano-indentation system, using the Berkovich indenter at a load of 100 mN and exposure time of 5s. Tribological sliding-friction tests were performed on the THT-S-BE-0000 tribometer using the standard «ball-disk» method according to the international standard ASTM G 133-95. It was determined that after PEH, the wear resistance of 0.34C-1Cr-1Ni-1Mo-Festeel increased by 3.4 times, and the microhardness increased by 2.6 times. Based on the study of the structure and phase composition, it was found that after PEH, a modified layer consisting of the α'-phase (martensite), γ'-phase, cementite M_3C and carbide $M_{23}C_6$ is formed. It is established that the bending-torsion of the crystal lattice is pure plastic ($\chi = \chi_{el}$), which does not lead to the formation of microcracks in the material. According to TEM studies, PEH steel 0.34 C-1Cr-1Ni-1Mo-Fe bring to the change of structural-phase state and the structure of the packet-plate martensite and the provision of small particles of cementite and carbide of $M_{23}C_6$ type uniformly located throughout the volume of the material. It is determined that the increase in microhardness and wear resistance of 0.34C-1Cr-1Ni-1Mo-Festeel after PEH. It is particularly related to the formation of martensite, as well as the formation of a defective substructure.

Biography

Bauyrzhan Korabayevich Rakhadilov (born March 28, 1988)PhD in Technical Physics, senior researcher of S.Amanzholov East Kazakhstan University. He is a specialist with a scientific background in the field of condensed matter physics and physical material science. The research activity of the principal investigatoris related to research on surface-plasma interactions, obtaining wear-resistant protective coatings, material modifications with concentrated energy flows. Winner of the State Scientific Scholarship for talented young scientists who made an outstanding contribution to the development of science and technology for 2013-2014 and for 2018-2019.

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Improving the reliability design of mechanical systems such as refrigerator

Seongwoo Woo
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To enhance the lifetime of mechanical system such as automobile, new reliability methodology – parametric Accelerated Life Testing (ALT) – suggests to produce the reliability quantitative (RQ) specifications—mission cycle—for identifying the design defects and modifying them. It incorporates: (1) a parametric ALT plan formed on system BX lifetime that will be X percent of the cumulated failure, (2) a load examination for ALT, (3) a customized parametric ALTs with the design alternatives, and (4) an assessment if the system design(s) fulfill the objective BX lifetime. So we suggest a BX life concept, life-stress (LS) model with a new effort idea, accelerated factor, and sample size equation. This new parametric ALT should help an engineer to discover the missing design parameters of the mechanical system influencing reliability in the design process. As the improper designs are experimentally identified, the mechanical system can recognize the reliability as computed by the growth in lifetime, LB, and the decrease in failure rate, λ. Consequently, companies can escape recalls due to the product failures from the marketplace. As an experiment instance, two cases were investigated: 1) problematic reciprocating compressors in the French-door refrigerators returned from the marketplace and 2) the redesign of hinge kit system (HKS) in a domestic refrigerator. After a customized parametric ALT, the mechanical systems such as compressor and HKS with design alternatives were anticipated to fulfill the lifetime – B1 life 10 years.

Biography

Seongwoo Woo has a BS and MS in Mechanical Engineering, and he has obtained PhD in Mechanical Engineering from Texas A&M. He major in energy system such as HVAC and its heat transfer, optimal design and control of refrigerator, reliability design of thermal components, and failure Analysis of thermal components in marketplace using the Non-destructive such as SEM & XRAY. In 1992.03–1997 he worked in Agency for Defense Development, Chinhae, South Korea, where he has researcher in charge of Development of Naval weapon System. He was working as a Senior Reliability Engineer in Refrigerator Division, Digital Appliance, SAMSUNG Electronics. Now he is working as associate professor in mechanical department, Addis Ababa Science & Technology University.

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Crystallographic basis of shape reversibility in shape memory alloys

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Firat University,Turkey

Shape memory alloys take place in a class of smart materials by exhibiting a peculiar property called shape memory effect. This property is characterized by the recoverability of two certain shapes of material at different conditions. Shape memory effect is based on dual crystallographic phase transformations, thermal and stress induced martensitic transformations in atomic scale. Thermal induced martensitic transformation occurs on cooling along with lattice twinning with cooperative movements of atoms in atomic scale, and ordered parent phase structures turn into twinned martensite structures. Product phase occurs as martensite variants with this transformation by means of the lattice invariant shears in <110> -type directions on the {110}-type planes of austenite matrix, and twinned martensite structures turn into the detwinned martensite structures by means of stress induced martensitic transformation by stressing material in the martensitic condition. Martensitic transformations have diffusionless character and movements of atoms are confined to inter atomic distances. Shape memory effect is initiated by successive cooling and deformation treatments, and activated thermally on heating and cooling. These alloys are plastically deformed in martensitic condition, with which strain energy is stored in the materials keeping the deformed shape, and released on heating by covering original shape on heating. These materials cycle between original and deformed shapes on heating and cooling, respectively in reversible shape memory effect in bulk level; whereas the crystal structure cycles between the twinned and ordered parent phase structures. Microstructural mechanisms responsible for the shape memory effect are the twinning and detwinning reactions. It is well known that twinning and detwinning play a considerable role in shape memory behaviour of materials. Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice invariant shears are not uniform in these alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on cooling. The long-period layered structures can be described by different unit cells as 3R, 9R or 18R, depending on the stacking sequences on the close-packed planes of the ordered lattice. The unit cell and periodicity is completed through 18 layers in direction z, in case of 18R martensite, and unit cells are not periodic in short range in direction z.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns reveal that both

alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation. X-ray diffractograms taken in a long time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result refers to a new transformation in diffusive manner.

Biography

Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post doctoral research scientist in 1986-1987, and studied on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has already been working as professor. He supervised 5 PhD- theses and 3 M.Sc- theses. He served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000.

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Long-acting injectable antipsychotics: Contemporary formulations and synthesis methods

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In the current treatment of the psychotic disorders, the prevention of the relapse observed inthe patients is a critical issue, which significantly improves the quality of life. Non-compliance to the oral medication or the lack of insight result in the increasedhospitalization rates. At this point, the long-acting injectable (LAI) antipsychotic drugs possess a therapeutic potential to obtain significantly fewer hospitalization rates and relapses ($p<.05$). The monthly injectables of the second-generation antipsychotics have indicated an improved efficacy together with the ability of slow release in the human body. The long-acting injectables of the second-generation antipsychotics such as olanzapine, paliperidone and risperidonediffer much in their formulations in comparison to the conventional ones.

LAI dosage form of olanzapine is the olanzapine pamoate preparation (Zyprexa Relprevv) is in theaqueoussolution; salt of olanzapineandpamoicacid is suspended in themicro-crystalline form. To produce the injectable formulation, the solvent extraction-evaporation route is used followed by filtration. After injecting the solution of the drug and polymer into the aqueous phase, the microspheres are obtained through the stirring and filtrating. In order to apply the freeze drying, it is required to be suspended in a vehicle. The paliperidonepalmitate preparation (marketed as InvegaSustenna) contains nanocrystal molecules in an aqueous suspension. From the synthesis aspect, the particle size of the nanocrystals determines the saturation solubility, based on the larger surface area. Due to the poor solubility, in preparing the formulation, the parenteral solution is obtained using the fatty acid ester of the drug. LAI dosage form of risperidone (Risperdal Consta) is infact, the encapsulation of risperidone into biodegradable polymeric microspheres. A biocompatible polymer is used for preparing the formulation, which has been approved to be used for the human due to its low toxicity.

The most common dosage forms of LAI require several techniques for the preparation of their formulations. In the present review, we will present an overview of the different synthesis methods used in these contemporary formulations and the major focus will be on the biodegradable polymeric microparticles, freeze/spray drying and the nanocrystal molecules related to the synthesis of LAI dosage forms of olanzapine, paliperidone and risperidone.

Biography

Burcu Ertuğis a materials scientist at the Faculty of Engineering and Architecture of Nişantaşı University. She has given various classes such as Materials Science, Building Materials, Manufacturing Processes, Engineering Mechanics at the Nişantaşı University and some other universities. She earned her PhD in Materials Science (Ceramics programme) from Istanbul Technical University (ITU) in 2008 and she completed her undergraduate studies at the same university. Her research topics are mainly in the medical field; the utilization of the ferrimagnetic properties in the cancer treatment, dental materials and their characterization (mechanical performance), nano-particles, glass-ceramics for dental applications. Particularly, she is interested in the psychology studies and the treatment of mental disorders.

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From metallic to semiconductor conversion of single –walled carbon nanotubes by chlorination

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In this research, the single-walled carbon nanotubes (SWCNTs) were treated with strong $HClO_4$ acid (98 %). The obtained doped nanotubes were investigated firstly by UV-vis-NIR absorption, Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy; and secondly by numerical calculations based on density functional theory (DFT) using generalized gradient and local density approximations (GGA and LDA) as implemented in SIESTA code. The results show significant changes in the behavior of metallic nanotubes. Indeed, a new pick attributed to the C-Cl stretching vibration was obtained in FTIR measurements, while the Breit-Wigner-Fano signature corresponding to the metallic character disappears from the Raman G-band. Secondly, the first-principles density functional theory calculations (GGA and LDA) show that the adsorption of chlorine atoms on the metallic (9, 9) carbon nanotubes wall (one Cl atom for 36 C atom) generates an energy gap in the electronic structure of these nanotubes, confirming the experimental results. This highlights a conversion of the metallic nanotube to semiconductor.

Biography

Mourad Berd is a senior lecturer in physics at the University of Bejaia in central eastern Algeria. He obtained his Ph.D. in materials physics at the University Mouloud Mameri of Tizi-Ouzou in collaboration with the CEMES -Toulouse – France. He worked on carbon nanotubes, fullerenes and peapods. He is interested in 2D materials and their composites as potential candidates for anode materials for Li-ion batteries or for hydrogen storage. For the last two years, he has been interested in ab. initio computational methods based on density functional theory using the computer code siesta for the study of nanomaterial properties.

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Hybrid drug nanoforms with metal nanoparticles in the controlled antibiotic drug delivery

Tatyana I. Shabatina[1], Olga I. Vernaya[1], YuriiN. Morosov[1], Alexander M. Semenov[2] and MichailYa. Melnikov[1]

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Cryochemical modification is a powerful method of reducing the size of drug substances particles, changing their form and crystal structure in order to improve their pharmaceutical properties. A possible application of this method allowed us to obtain antibiotics nanocrystals and hybrid nanoforms of metal particles and drug substances. The use of antibiotics and other antimicrobial agents in medicine has led to the emergence of many resistant strains of microorganisms. This problem is solved by the synthesis of new antibiotic substances and simultaneous use of hybrid nanoforms of antibiotics and metals nanoparticles. Antibacterial compositions were produced by low temperature freeze drying technique of water solution containing metal nanoparticles and antibacterial components. The thorough investigations TEM, electron microdiffraction, Fourier transformation infrared spectroscopy (FTIR), UV absorption spectroscopy, X-ray diffraction, differential thermal analysis (DTA) were made, It was shown that the hybrid compositions were including Ag,Cuand Fe/or metal oxide nanoparticles of 5-70 nm in diameter and nanoparticles of antibiotics of 50-350 nm in diameter. Drug cryoforms possessed modified crystal structures and lower melting temperatures, New cryoformed hybrid compositions of nanosized metal and antibiotic particles demonstrates higher antibacterial activity against *E. coli 52, S.aureus 144, M. cyaneum 98, B. cereus 9* compared to the original drug substance and individual metal nanoparticles. Cryomodified forms of dioxidine and hentamicine, as also hybrid nanoforms of these antibacterial substances with metal nanoparticles have been included in polymer filmsofpolyvinyl alhogol (PVA), polyvinylpyrrolidone (PPV) and gelatine. It was shown the possibility of directed delivery and controlled release of antimicrobial components, as also higher biomedical activity of hybrid nanoforms against *E. coli 52, S.cureus 144* compared to the individual components.

Biography

Tatyana I. Shabatina wasgraduated with honor in 1978 from Department of Chemistry, Moscow State University, in 1984 received Ph.D. in Physical Chemistry, Department of Chemistry, Moscow State University, title of work: Dimerization of nitrosocompounds and photoinduced nitroxide radicals formation in nematic liquid crystals, under supervision of Prof. Gleb B. Sergeev, in 2013 became Doctor of Chemical Sciences, specialization in Physical Chemistry, Department of Chemistry, Moscow State University, title of work "Molecular association and cryoformation of hybrid metal-mesogenic nanosystems with controlled morphology and structure". From 2014 till now – Head of the Laboratory on Low Temperature Chemistry at Department of Chemistry M.V. Lomonosov Moscow State University. 1994 - research training at Max-Plank Institute, Muelheim (Germany), 1996 –research training in the University of Amsterdam (Nederland), 2000 – research visit in the Kansas State University (USA), 2009 – Visiting Professor, exchange visit in the University of York (UK).Research interests: NanoChemistry, Cryochemistry, Hybrid Metal-Mesogenic Nanosystems, Nanostructured Films, Nanoforms of Drugs, Nanosized Metals, Spectroscopy at Low Temperatures.

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The effect of functional additives on the structure and properties of PHB-based nanofibers

P. Tyubaeva[1,2], A. Olkhov[1,2], A. Lobanov[1,2] and **A. Popov[1,2]**

[1]Plekhanov Russian University of Economics institute, Russian Federation
[2]Russian Academy of Sciences, Russian Federation

Highly porous polymer carriers of biologically active substances are currently widely used in biology and medicine as long-acting matrices, matrices for cell engineering, antibacterial therapeutic systems, matrices for controlled release of drugs, etc. The study of the design possibilities and the directed influence on the structure and properties of semi-crystalline polymers of natural origin using various additives and modifiers is an area of a great interest in our days.Thus, various functional additives, including porphyrin complexes with various metals, are used to create biocompatible antibacterial polymer systems. The aim of the work was to study the effects of zinc (ZnTPP), manganese (MnClTPP) and iron (FeClTPP) tetraphenylporphyrin complexes on the supramolecular structure and properties of the electrospun fibers based on the biopolymer polyhydroxybutyrate (PHB). Various methods were used for studying the structure and properties of the materials, including DSC, EPR, TGA, mechanical analysis and microscopy methods. In the work, significant differences in the structure of PHB with 1-5 wt. % of the FeClTPP, ZnTPP, and MnClTPP complexes were found. The influence of the complexes on the morphology, mechanical and diffusion properties, the kinetics of biodegradation of non-woven materials was established. Special attention was paid to the studying of the antibacterial activity and the rate of biodegradation of the obtained materials. An approach for solving the actual problem of the formation of fibers of certain morphology with a set of necessary operational properties is proposed.

Biography

Tyubaeva Polina graduated from Plekhanov University of Economics in 2015 with a degree in commodity science and commodity research, graduated from the Institute of Biochemical Physics in 2019 with a degree in chemical physics, got a PhD. in chemistry in 2020. Main research interests: electrospinning of biopolymer materials, creation of innovative biocompatible therapeutic systems with special properties.

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Biodegradable polymers based on polyolefins and elastomers

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The development of biodegradable polymers that can be readily degraded by common types of microorganisms (bacteria, fungi, etc.) is of great importance. A promising strategy for achieving this goal is the inclusion of natural additives into the synthetic polymer matrix, which provide a nutrient medium for attracting microorganisms to the polymer surface and thereby initiate the process of its biodegradation. Here we present the results of our study on the use of natural rubber as an additive to low-density polyethylene in order to create a polymer compound for rapid biodegradation in soil. Polymer blends based on polyethylene with a natural rubber content of 0 to 50 (wt.%) were obtained by mixing and pressing the ingredients at elevated temperatures, followed by rapid cooling. To study the biodegradation process, the samples were placed in laboratory soil and the degree of degradation was assessed by the amount of weight loss over time. The physical and chemical properties of the samples were monitored by several methods, including tensile testing, optical microscopy, differential scanning calorimetry, Fourier transform infrared spectroscopy, and others. It has been shown that the presence of natural rubber significantly increases the decomposition rate of the polyethylene-based composites. The greatest effect is observed for samples with a natural rubber content of 50 (wt%). For these samples, the weight loss was more than 40% of the original weight during the time of experiment. Also, on the basis of a comprehensive study of the physical and chemical properties, it was shown that all studied samples of polymer composites based on polyethylene with natural rubber additives have satisfactory mechanical properties sufficient for use as a packaging material. Thus, we conclude that the use of natural rubber as an additive is an effective method for the production of biodegradable materials based on polyethylene.

Biography

Ivetta Varyanis a Russian chemist specializing in biodegradable polymers and composites. She studies the influence of external factors (mechanical stress, chemical modification, oxidation, impurities and additives) on the structure, molecular dynamics of polymers and composite materials based on low-density polyethylene with natural rubber additives. She is currently a researcher at a number of institutions, including the Laboratory of Physics and Chemistry of Compositions of Synthetic and Natural Polymers of the Institute of Biochemical Physics, Russian Academy of Sciences and the Center for Collective Use of Plekhanov Russian University of Economics. Also, with the assistance of Ivetta Varyan, in 2021, the Center of the National Technological Initiative was established in the direction of "Technologies for Modeling and Development of Materials with Specified Properties". In 2015 she graduated with honors from Plekhanov Russian University of Economics. In 2020 she completed her postgraduate studies in the specialty "high molecular weight compounds".

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Modern elastomers using anisotropic carbon based fillers

U. Giese

German Institute of Rubber Technology, Germany

Modern elastomers used in several technical applications should fulfil increasing requirements like especially concerning heat stability, media stability, permeation behavior, electrical conductivity, strength and abrasion properties. Beside the selection of an appropriate polymer, an improved cross linking system and other additives, the fillers play an important role. Nano-scaled materials like carbon nanotubes (CNT), nano-graphite nanoG), graphene platelets (GNP), graphenes and carbon-nanohorns (CNH) are fillers with high potential, caused by high specific surfaces and spheric porous or high aspect ratio morphologies. In the presented work high sophisticated raw materials like CNTs, different GNP-materials and carbonanohorns are characterized for their morphology, specific surfaces and adsorption properties.Rubber compunds containing such fillers are prepared using polyisoprene (IR), nitrile-butadiene rubber (NBR), fluoro rubbers (FKM styrene-butadiene rubber (SBR) and slightly epox. (~9%) SBR or NR. The compounds were characterized for viscosity, vulcanization behaviour, physicals, electrical conductivity and for the filler-polymer interaction by swelling experiments. All investigations are carried out in comparison to traditional used carbon black. Some modifications of the fillers like GNP (commercial type xgC50) were done by oxidation and esterification with the intention to improve the polymer –filler interaction for example in butyl rubber compounds (BIIR).

Biography

Ulrich Giese received his PHD in chemistry from the University of Paderborn/Germany in 1988. He started in 1989 working in rubber research and chemistry at the German Institute of Rubber Technology (DIK e.V.). Currently he is Managing Director of the DIK e.V. and of the new founded "DIK Testing Laboratory" with overall 40 scientists and 35 technicians. Furthermore U. Giese developed the DIK activities in teaching and education. Since 2010 U. Giese is a distinguished professor at the Leibniz University of Hannover (faculty of natural science: resp.: "Applicated Polymer Chemistry".) Since 2013 he is editor for the scientific part of the international Rubber Journal "Kautschuk Gummi Kunststoffe".

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Theme: Navigating the future research directions in the field of Materials Science and Engineering

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Modeling and simulation of micro-structural material properties and reactive injection moulding in polyurethane foams

K. Steiner, M. Kabel, D. Niedziela, S. Rief and **H. Andrä**

Fraunhofer Institute for Applied Mathematics ITWM, Germany

Products made of polyurethane foam are manufactured by the chemical reaction of various low-viscosity raw materials and additives. The diversity of different formulations to meet the requirements of the market makes the characterization of their processing and final product quality important for a simple and error-free production. The modeling and simulation of such processes as well as the detailed analysis of the resulting material properties are equally of great importance. This provides additional findings without the expense of real tests and makes it easier to design components.

The talk will present modeling and simulation techniques carried out against this background. On one hand, we will demonstrate simulation tools and their application to perform virtual micro structural analysis of PU foam structures to characterize the mechanical and fluid dynamical properties of different foams. Especially, the material performance like flow resistivity, acoustic absorption and stability under different compression situation will be studied which depends strongly on the local foam density.

On the other hand, we explain a mathematically model to simulate the reactive injections moulding process for the foam expansion. The reactive multiphase model parameters are automatically identified from well know tube expansion experiments. The simulation results in detailed information about the filling behavior and the foam density and temperature distribution during and at the final state of the injection process. The simulation tool FOAM can be applied for all kinds of PU foams as well as for quite different manufacturing applications (car seats, refrigerator, insulation panels and fiber reinforced sandwich structure) to optimize the layout, the injections paths or the venting positions.

Finally, we will show how the two methods can be combined to o create a digital twin for foam components in the future.

Biography

Konrad Steiner a member of the Department Flow and Material Simulation at Fraunhofer ITWM in Kaiserslautern Germany. The strength of the department is the resident expertise in company-specific software solutions and the development, supply, and specific use of multi-scale and multi-physics methods suitable for industrial application. Our simulation tools combine actual research results of model reduction methods, automatic parameter identification and machine learning to increase efficiency. He is an Expert of Comp. Fluid Dynamics and Microstructure Simulation.

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How to test the arrhenius validity of elastomers during ageing

M. Zaghdoudi, M. Jaunich, A. Kömmling and **D. Wolff**

Bundesanstalt für Materialforschung und -prüfung (BAM), Germany

The main task of the division "Safety of Storage Containers" at BAM is the safety assessment of storage containers for radioactive waste. A sufficient sealing of bolted lid systems for the safe containment of the waste for transport, storage and disposal is very important. Extensive knowledge of the change of the elastomer's properties during ageing and the availability of reliable end-of-lifetime criteria is mandatory to guarantee long term safe enclosure.

In a long-term test programme over 5 years we have studied the degradation and the change of sealing properties of several elastomers, including EPDM, at four different ageing temperatures (75°C, 100°C, 125°C and 150°C). Compression stress relaxation (CSR) and compression set (CS) experiments were carried out. It has been found that when the data does not cover a sufficient time frame necessary for the evolution of the degradation of a chosen property, a curvature in the Arrhenius relationship is observed. For CSR, the curvature was observed for samples aged up to 186 days. As for CS experiments, the curvature was detected for sample aged up to 2 years. To cover the possible lack of experimental long-term data at low temperatures, a numerical model for CSR was developed and longer ageing times for the simulation were adopted. A degradation-rate based model for the evolution of degradative processes is proposed. The main advantage of the model is the possibility to quickly validate the interpolation at lower temperatures within the range of slower chemical processes without forcing an Arrhenius straight-line extrapolation. The model was also applied to CS experiments and validated by the 5 years experimental results where the curvature was gone, and the degradation property has followed an Arrhenius relationship. The contribution of the two degradative processes are shown over CS and CSR respectively.

Biography

Maha Zaghdoudi obtained her PhD in mechanics and processes with the focus on modelling and experimental investigations of elastomer behaviour. She works at the Bundesanstalt für Materialforschung und -prüfung (BAM), Germany, in Department 3 Containment Systems for Dangerous Goods, Division 3.4 Safety of Storage Containers. Her research field is in polymer science and materials engineering (testing and modelling). Her current research focus is the investigation of rubber seals used under different thermo mechanical conditions and for long time periods.

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Insights into the bead fusion mechanism of expanded polybutylene terephthalate (E-PBT)

H. Ruckdaeschel, D. Raps, T. Standau, M. Luik, V. Altstädt and **J.Kuhnigk**
University of Bayreuth, Germany

Expandable polystyrene (EPS) and expanded polypropylene (EPP) dominate the bead foam market. As the low thermal performance of EPS and EPP limits application at elevated temperatures novel solutions such as expanded polybutylene terephthalate (E-PBT) are gaining importance. To produce parts, individual beads are typically molded by hot steam. While molding of EPP is well-understood and related to two distinct melting temperatures, the mechanisms of E-PBT are different. E-PBT shows only one melting peak and can surprisingly only be molded when adding chain extender (CE). This publication therefore aims to understand the impact of thermal properties of E-PBT on its molding behavior. Detailed differential scanning calorimetry was performed on neat and chain extended E-PBT. The incorporation of CE remarkably reduces the crystallization and re-crystallization rate. As a consequence, the time available for inter diffusion of chains across neighboring beads increases and facilitates crystallization across the bead interface. For E-PBT bead foams, it is concluded that sufficient time for polymer inter diffusion during molding is crucial and requires adjusted crystallization kinetics.

Biography

Since January 2021, Prof. Dr.-Ing. Holger Ruckdaeschel is full professor for Polymer Engineering at University of Bayreuth. Based on his strong academic background, he became member of various institutes in recent time, for instance the Bavarian Polymer Institute. He is also well-connected to multiple companies and industries. Before becoming professor, he has been working at BASF for 13 years. In his current role, he is connecting material, technology and application. His primary material research areas are resins & composites, polymer foams, functional thermoplastics and integrative as well as additive manufacturing. He integrates the aspects of digitalization and sustainability into research to develop a modern approach for polymer science & engineering.

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Time optimization of seed-mediated gold nanotriangle synthesis based on kinetic studies

E. Podlesnaia, A. Csáki and **W. Fritzsche**
Leibniz Institute of Photonic Technology (IPHT), Germany

Plasmonic nanoparticles have become important materials due to their special optical properties and development of optic and photonic technologies. In various application fields (e.g. plasmonic sensor technology) the shape anisotropic nanoparticles are of vast interest. That makes the synthesis of such structures to appear frequently in the focus of research. We report the kinetic studies of the gold nanotriangle synthesis. *In situ* measurement of the reaction mixture UV-Vis properties was utilized as a powerful tool for monitoring the evolution of synthesis at each step. The obtained data, in combination with the knowledge of occurring chemical processes, allowed to rationally determine the time intervals required for successful reproduction of the procedure and shortening it from three days to one. The samples synthesized with following each protocol were evaluated with UV-Vis spectroscopy and SEM imaging. Analysis of the obtained data revealed no significant differences in such quality characteristics as shape yield and size distribution. Besides the practical interest of time consumption optimizing, this study represents an example of how characterization approaches can be utilized to determine the critical durations of key synthesis steps in order to improve the efficiency of nanoparticle production.

Biography

Ekaterina Podlesnaia, PhD student in the workgroup Nanobiophotonics at the Leibniz- Institute of Photonic Technology (Leibniz-IPHT) studied chemistry at the Southern Federal University (SFedU, Rostov-on-Don, Russia). She received her diploma in Chemistry in 2019 and currently works in the field of physical chemistry and nanomaterials..

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Strengthening aluminium alloys under as-cast condition for high pressure die casting

Shouxun Ji, Xiangzhen Zhu and **Xixi Dong**
Brunel University, United Kingdom

Lightweight materials and structural manufacturing require castings to have high strength and thin wall structure. Therefore, the strength increase of high pressure die castings is critical for industrial applications. However, most of the high pressure die cast parts are not suitable for further strengthening by solution and ageing heat treatment due to blistering. Although the recently developed vacuum-assisted high pressure die cast is a way to produce heat treatable die-castings, extra time and energy costs are associated in the production. Therefore, most of the high pressure die cast parts are preferred to be applied under as-cast condition.

Starting from the review of strengthening mechanisms, the present paper aims to introduce the recent development of new aluminium alloys for improving the as-cast strength with high pressure die casting. The as-cast alloys with different approaches can offer the yield strength greater than 220 MPa and the tensile strength greater than 390 MPa, as well as the industrially acceptable elongation greater than 4%, showing the great potential in industrial applications because of the equivalent cost in comparison with the existing popular alloys.

On top of the study in composition optimization and strengthening mechanisms, the industrial trials with real engineering components will be introduced to verify the improvement of new development.

Biography

Shouxun Ji is a research team for lightweight alloys and structures at Brunel University London. He has 23 registered patents in WO, EU, UK, and CN on aluminium alloys, magnesium alloys, casting processes including semi-solid process, high pressure die casting, low pressure die casting, centrifugal casting, sand casting and metallurgical equipment. He is the PI and CoIof more than 20 projects from EPSRC, Innovate UK, APC and UK&EU industries. He is a technical committee member in several organizations, including NFE035 Light Metals and their Alloys, BSI international, UK; ISO/TC 079/SC07 'Aluminium and cast aluminium alloys'; ISO/TC 079/SC06 'Wrought aluminium and aluminium alloys'; ISO/TC 079/SC05 'Magnesium and alloys of cast or wrought magnesium'.

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Emerging non-volatile electronic memory devices from polymers to transition metal oxides

Iulia Salaoru

De Montfort University, United Kingdom

In recent years, the interest in non-volatile memory (NVM) has shown a rapid increase from both perspective academia and industry. The factors driving this intense interest are mainly attributed to their simple (two-terminal), zero power draw for sustaining a state, high-speed operation, good endurance but also their multi-state capacity. Solid state implementations of these devices show great potential in applications such as: reconfigurable architectures, neuromorphic computing and artificial synapses. Numerous candidates for emerging electronic memory technologies such as ferroelectric (FeRAM), phase-change random access memory (PCRAM), magneto-resistive (MRAM), resistive random-access memory (ReRAM) and organic memory have been proposed and investigated by a number of research groups worldwide. The main functional property of NVM cells is switching between distinct electrical resisitive states on application of distinct SET and RESET potentials, with a state being sensed by an intermediate READ voltage. Current research efforts are focused on determining the physical switching mechanism that facilitates the switching behaviour particular in ReRAM based on transition metals and polymer memory devices.

This talk will encompass two of the most investigated non-volatile memories: polymer and transition metal oxide resistive memory. The possible physical switching/charging mechanism(s) along with experimental evidence will be presented in this work. Along with the electrical experimental results, we have also used the chemical characterization tools to further understand the operating mechanism, will likewise be discussed.

Biography

Iulia Salaoru received a BSc (Physics), MSc (Physics) degree from the "Al. I. Cuza" University, Iasi, Romania, where she also awarded a PhD degree for her work on AIIBVI semiconducting compounds. Since completing her PhD, she has worked as a Postdoctoral Researcher at: Mechanics of Materials Research Group, Department of Engineering, University of Leicester; Emerging Technologies Research Centre, De Montfort University, Leicester; Centre for Bio-inspired Technology, Imperial College London; Nanofabrication Centre, University of Southampton and Warwick Manufacturing Group (WMG), University of Warwick. Currently, he is a Senior Lecturer in Engineering and Sustainable Development, Faculty of Computing, Engineering and Media at De Montfort University, Leicester, UK.

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A hierarchical bayesian calibration of data-driven models for composite laminate consolidation

N. Papadimas[1], J. Bennett[1], A. Sakhaei[2] and T. Dodwell[1,3]

[1]University of Exeter, United Kingdom
[2]University of Kent, United Kingdom
[3]The Alan Turing Institute, United Kingdom

Composite modelling of consolidation processes is playing an important role in process and part design, by indicating the formation of possible unwanted defects (e.g. wrinkles(Dodwell, 2014)) prior to expensive experimental iterative trial and development programmes. Composite material in their uncured state display complex constitutive behaviour, which has received much academic interest, and with this different models have been proposed ((Gutowski T. G., 1987),(Gutowski T. G., 1987),(Hubert, 1999),(Li, 2002),(Sakhaei, 2020)). Errors from both the modelling assumptions and statistical variability which arise from the fitting of constitutive material models will propagate through any simulation in which the material model is used, leading to uncertainty in predictions.

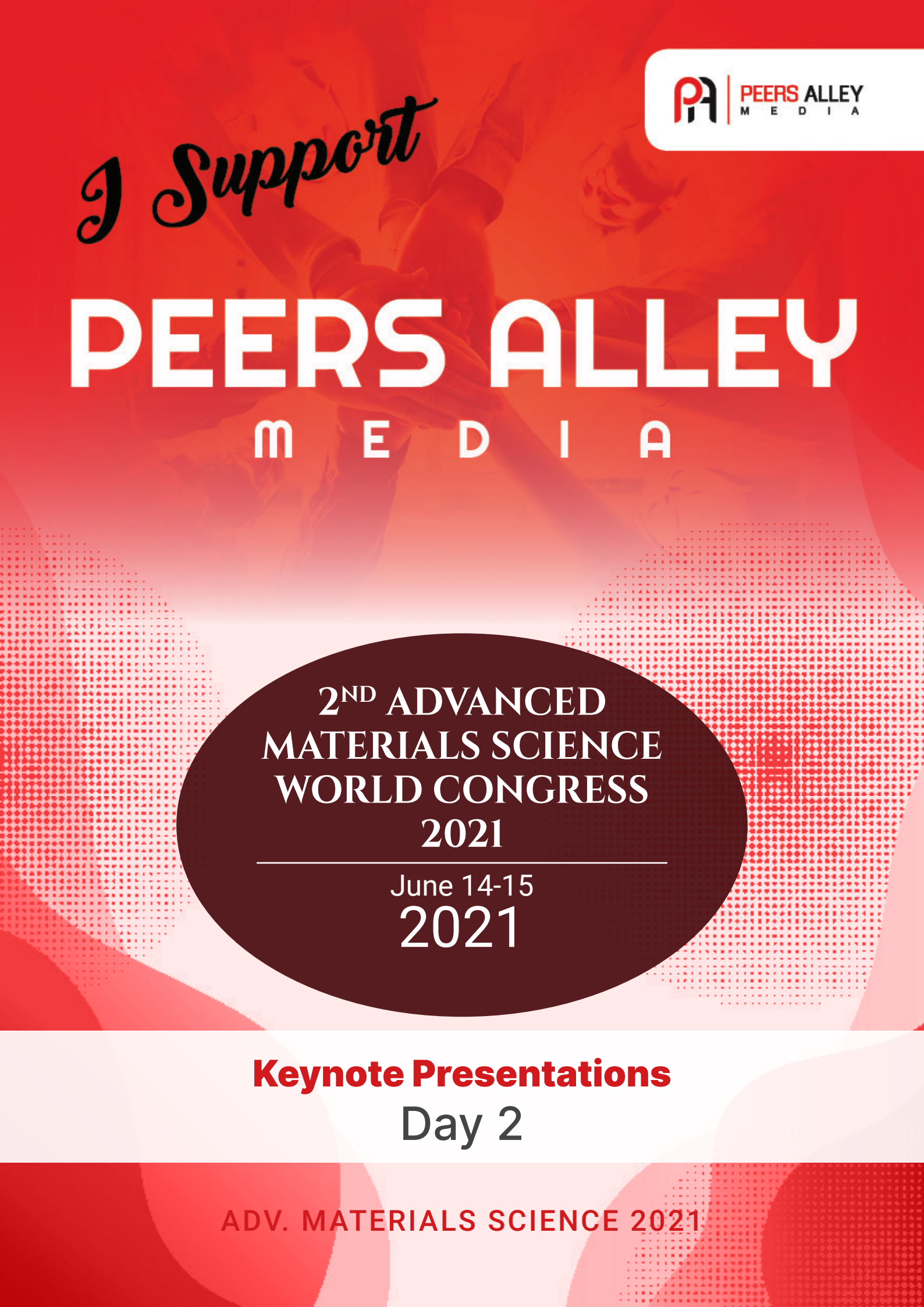
We propose a general hyperelastic polynomial representation, which can be readily implemented in various nonlinear finite element packages. In our case we choose, FEniCS(M.S Alnes, 2015). The coefficients are assumed uncertain, and therefore the distribution of parameters learnt using Bayesian inference, more explicitly Markov Chain Monte Carlo (MCMC) methods. In engineering the approach often followed is to select a single set of model parameters, which on average, best fits a set of experiments. There are good statistical reasons why this is not a rigorous approach to take.

To overcome these challenges, we propose a hierarchical Bayesian framework (Gelman, 2013) in which population distribution of model parameters is inferred from an ensemble of experiments tests. The resulting sampled distribution of hyperparameters, are approximated using Maximum Entropy methods, so that the distribution of samples can be readily sampled when embedded within a stochastic finite element simulation at higher length scales.

The methodology is validated and demonstrated on a set of consolidation experiments of AS4/8852 with various stacking sequences. The resulting distributions are then applied to a stochastic finite element simulations of the consolidation of curved part, leading to a distribution of possible model outputs. With this, the paper, as far as the authors are aware, represents the first stochastic finite element implementation in composite process modelling.

Biography

Nikolaos Papadimas is a PhD candidate in his 3rd year of studies who focus on Data Driven models, uncertainty quantification and machine learning methods applied in Composite material processes.



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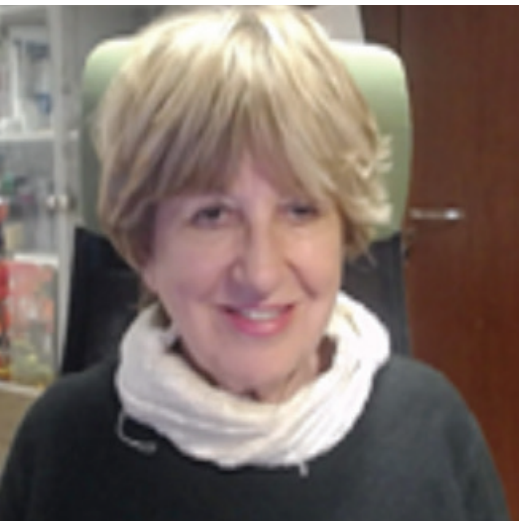

BIOGRAPHY

Spomenka Kobe is Scientific Advisor, Department for Nanostructured materials, was 16 years acting as a Head of the department. She is a full professor at the International Postgraduate School "Jožef Stefan" and was for 20 years the Leader of the National Research Programme. Until 2017 she was the Slovene director of The International Associated Laboratory between CNRS, Nancy, France, and Jožef Stefan Institute, Ljubljana, Slovenia. She is a member of the Slovenian Academy of Engineering. In 2019 she was the recipient of the prestigious *Fray International Sustainability Award* for "Leadership in development new technologies that contribute to global sustainable development in the environment, economy, and social points of view."

S. Kobe

Jožef Stefan Institute, Slovenia

RE-based magnetic materials for e-mobility

Rare-Earth Transition Metals permanent magnets are vital components in the rapidly-developing renewable energy sector, where the motors require strong magnets with the ability to operate at temperatures well above 100°C. To achieve high coercivity, remanence, and, consequently, high energy product at elevated temperatures, the addition of a heavy rare earth (HRE) to the basic Nd-Fe-B composition is needed. HRE are on the very top of the list of Critical Raw Materials.

In our first goal to drastically reduce the use of HRE, we focused on developing a new method, which enabled us to achieve the properties needed for high-temperature applications with the lowest amount of scarce elements. Now, we are focusing on recycling end-of-life magnets EoL to minimize European dependence on China. We managed to minimize the amount of HRE used, down to 0.2 at %, while the improvement of coercivity was 30% with minimal loss in remanence by developing new inventive techniques further transferred to pilot production. 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 a clean environment. The results presented are based on different processing method sand are focused on studying the mechanism for upgrading the magnetic properties of standard and recycled EoL NdFeB magnets in tailoring the microstructure, phase ratio, and phase composition. They are obtained in the frame of four EU-funded projects, ROMEO (finished), REProMag (finished), MaXycle, and SUSMAGPRO (running). The use of newly developed high energy magnets with a minimum amount of HRE and by using a highly effective HPMS process (Hydrogen Processing of Magnetic Scrap) for recycling is envisaged to enable a circular economy ecosystem for NdFeB magnets in renewable energy and e-mobility sectors.

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BIOGRAPHY

A. Łukaszczyk is an Assistant Professor at the AGH-University of Science and Technology in Cracow. Her research focuses on electrochemical and corrosion behavior of biomaterials e.g. stainless steels, titanium and its alloys, cobalt-based alloys, NiTi alloys etc. She received her M.Sc. in Chemistry from the University of Technology in Cracow and her Ph.D. in the field of Metallurgy from the AGH-University od Science and Technology in Cracow.

A. Łukaszczyk

AGH University of Science and Technology, Poland

Electrochemical corrosion resistance of polyetheretherketone-based coatings electrophoretically deposited on the Ti-6Al-4V alloy

Titanium and its alloys are often used as structural components in the aerospace, automotive, petrochemical, marine industries, chemical and biomedical engineering. A major disadvantage of all titanium alloys, especially in applications exposed to friction are their poor resistance to abrasive wear, high tendency to seize, high coefficient of friction (COF) and relatively low hardness. In consequence, the corrosion resistance of these alloys was also decreased and in the case of orthopaedic implants, the inflammation phenomena around implants can occur in a long time. Hence, the improvement of the surface properties is a major challenge. The aim of this work was to investigate the electrochemical corrosion resistance of the composite polyetheretherketone PEEK-based coatings, TiN/PEEK and graphite/PEEK, deposited on Ti-6Al-4V titanium alloy substrates. The coatings were fabricated by electrophoretic deposition (EPD) and heat treatment. The microstructure of coatings was investigated by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffractometry (XRD). The scratch resistance and tribological properties were also studied. Post-EPD heat treatment densified the coatings and changed the PEEK structure from amorphous into semi-crystalline. Both coatings were characterized by very good scratch resistance. They reduced the coefficient of friction and increased wear resistance of the alloy during dry sliding contact with alumina ball. The corrosion studies(open circuit potential, linear sweep voltamperometry, electrochemical impedance spectroscopy) demonstrated that the composite PEEK-based coatings enhanced electrochemical corrosion resistance of the alloy in aqueous solutions containing ions of chloride.

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Matjaž Godec has completed his Ph.D at University of Ljubljana, Slovenia, at Faculty of Natural Science and Engineering, Metallurgy in 1997. Since 2011, he has been a director of Institute of Metals and Technology in Ljubljana Slovenia. Currently, he is a head of national research programme Physics and Chemistry of Metallic Materials and of two projects both dealing with additive manufacturing. He is an expert member at the advisory body Steel Advisory Group within the Research Fund for Coal and Steel as the representative of Slovenia, which falls under the umbrella of the European Commission's Directorate general for Research and Innovation.

M. Godec

Institute of Metals and Technology, Slovenia

Influence of coupling two additive manufacturing technologies on the microstructure of Nickel alloys

The two most common additive-manufacturing technologies are powder-bed fusion (PBF) and direct-energy deposition (DED), each of which has some advantages and disadvantages. PBF allows the processing of very complex parts with good microstructures, while DED allows rapid processing, but with coarser microstructures. For many applications where only a small portion of the part is complex and the rest is larger and geometrically simple, combining the two technologies can be a very effective way to rapidly manufacture such parts. Possible applications include those based on nickel alloys, where it is important to control the precipitates the during additive manufacturing as well as during the subsequent heat treatment. In this study, we focused on achieving of the appropriate microstructures for different nickel alloys and the related mechanical properties. Attention was also paid to the bonding of such hybrid additive-manufactured parts.

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Grain-boundary segregation of boron in high-strength steel: Characterization and modelling

P. Maugis[1], G. Da Rosa[1,2], A. Portavoce[1], J. Drillet[2], N. Valle[3], E. Lentzen[3] and **K. Hoummada[1]**

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[2]ArcelorMittal Maizières Research SA, France
[3]Luxembourg Institute of Science and Technology, Luxembourg

Adding small amounts of boron in low-carbon steels has a positive effect on hardenability. This is commonly explained by boron segregation at prior austenite grain boundaries delaying the austeniteto ferrite phase transformation during cooling, or during isothermal bainitic transformation. We investigated boron segregation at austenite grain boundaries after soaking in a high-strength low-carbon steel using high resolution secondary ion mass spectrometry (nano-SIMS) and atom probe tomography (APT). We found that boron segregation at grain boundaries increases with the soaking temperature. This is due to boride precipitate dissolution, which increases the amount of solute boron in the grains. Using a finite difference modeling of the Onsager equation for diffusion, together with the hypothesis of local equilibrium at the grain boundaries, it was possible to fit the concentration profiles of boron in the vicinity of the grain boundaries. The diffusion coefficient and this gregation enthalpy of boron were identified. These results have important practical consequences for controlling the levels of segregated boron in steels.

Biography

Philippe Maugis has been working for 13 years in the steel industry in ArcelorMittal research center at Maizières-lès-Metz, France. Since 2010, he is full professor at Aix-Marseille University. His main interests are related to the microstructural evolutions of high-strength steels, including phase transformations, precipitation, recrystallization and solute segregation at structural defects. He specializes in physical modelling at all space scales (DFT, Monte Carlo, Mean-field models).

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Repair of components using additive manufacturing technologies

W. Pacquentin[1], T. Cailloux[1], J. Varlet[1], G. Rolland[2], P. Widen[3] and H. Maskrot[1]
[1,3]Université Paris-Saclay, France
[2]EDF – R&D, France

Direct Laser Deposition (DLD) is a versatile, cost-effective and time-saving tool to repair worn out or damaged parts compatible with a vast panel of metals and complex geometries. In-situ repairing of a component part of a large scale structure may save the complexity of disassembling the host structure using a robot arm to convey the laser beam and the metal powder carrying gas feed. Process parameters include laser beam and powder jet characteristics as well as raster scan strategies and part preparation protocol. The search for the adequate parameter set is at the heart of R&D. For nuclear applications, cobalt-based hardfacing coatings are repaired in spite of their sensitivity to crack formation induced by extensive thermal cycling. For naval applications, we successfully repaired a SS316L sample by restoring its initial corrosion resistance. Samples were made using induction-heating assisted DLD and characterized by non-destructive testing, microstructural examinations, mechanical tests and corrosion evaluation performance. The quality criteria (dense deposition, minimum porosity and absence of crack) are met.

Biography

Wilfried Pacquentin received his M.Sc. in Materials Science from Université Paris XII and a Ph.D. degree in Physical chemistry from Universityof Burgundy France. He then joined the French Alternative Energies and Atomic Energy Commission (CEA), now a division of *Université Paris-Saclay,* as a scientist in the field of materials processing using lasers. He initially developed laser surface treatments of nuclear materials for decontamination, improvement of corrosion resistance or diffusion coating. His interests gradually broadened towards additive manufacturing technologies applied to functionally graded materials, advanced coatings, maintenance and repair.

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A greener approach to the solution combustion synthesis of mixed oxides: Role of the chemical precursors

F. Deganello

Italian National Research Council, Italy

Nowadays, advanced materials production needs to rely on sustainable synthesis procedures. In order to be sustainable, a synthesis procedure should be (I) efficient (cost-saving, energy-saving, time-saving), (II) eco-friendly, (III) scalable, (IV) reproducible and (v) beneficial for environment, society and economy. Solution combustion synthesis (SCS) is a well-known chemical methodology for the powerful and versatile preparation of mixed oxides, based on the self-sustaining redox reaction between fuel and oxidant in the presence of metal precursors. SCS satisfies most of the sustainability requirements cited above, although not all of them. In fact, a greener approach is necessary in order to call this methodology as sustainable. This mini-plenary presentation highlights the steps towards a greener approach to SCS, from the chemical precursors to the materials application.

The first step is the use of waste-derived resources for fuels or metal precursors. A further step is an improvement in efficiency, scalability and reproducibility of SCS, which is possible only through a profound knowledge of the relationships between synthesis parameters and final properties of the obtained materials. In this respect, the chemical composition of the material plays an important role and it should be taken into account during optimization of the synthesis parameters. The use of several complementary characterization tools is highly recommended, for a deeper understanding of all the effects caused by the synthesis parameters. Finally, the applicability of the material for the benefit of the environment (I.e. pollution control; waste re-use), society (i.e.: clean water, clean air or clean energy production/accumulation) and economy (i.e.: circular economy; higher efficiency of the industrial synthesis processes) fulfills the last requirement. All these considerations refer to SCS, although most of them can be easily extended to other chemical methodologies for the preparation of mixed oxides.

Biography

Francesca Deganello is research chemistat CNR-ISMN (Istituto per lo Studio dei Materiali Nanostrutturati) in Palermo (Italy)since 2001.She obtained degree in Chemistry and PhD in Chemical Sciences at Università degli Studi di Palermo, Italy. She visited national and international laboratories like for example Trieste University (Italy), Tokyo University (Japan) and INRS-EMT (Canada). Her current research interests concern the sustainable synthesis of nonmaterial's for energy and environmental applications. She is responsible for the ISMN unit of international projects concerning the wastewater pollutants abatement. She is scientific tutor/co-tutor of undergraduate, PhD and Post.Doc students. She also deals with the communication and dissemination of Chemistry for schools and public and performs reviewing and editorial activity for materials-related journals.

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On the interaction of carbon nanotubes with photosynthetic assembles

M.D. Lambreva[5], A.A. Volgusheva[1], P. Akhtar[2], P.H.Lambrev[2], S. Orlanducci[3], A. Margonelli[4], G. Sipka[2] and T.K. Antal[1]

[1]Moscow State University, Russian Federation
[2]Hungarian Academy of Sciences, Hungary
[3]University of Rome Tor Vergata, Italy
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The development of various bio hybrid natural or artificial systems for promotingthe solar energy conversion is of high priority in contemporary energy research. It has been suggested that single-walled carbon nanotubes (CNTs) might boost photosynthetic activity by enlarging the light spectrum region available for the photosynthetic reactions (Nat.Mater.2014, 13:400-408). The actual mechanism of this phenomenon is still unclear and the limited number of studies dealing with the CNT interplay with photosynthetic complexes provided controversial indications including both energy/charge transfers forward and from the nanotubes.

We have evaluated the potential of CNTs to enhance the photosynthetic performance of microalgae and thus to open new opportunities for more efficient use of the photosynthesis-based systems in the sustainable production of energy, biomass and high-value compounds. Our studies of the effects of CNTs on the photochemical reactions in the unicellular green algae Chlamydomonas reinhardtii pointed out the ability of the nanotubes to modify the growth and photosynthesis of the algal cells. Particularly, the characterisation of CNT interaction with photochemical events occurring in photosystem II (PSII) and photosystem Ivia chlorophyll fluorescence spectroscopy indicated CNT-induced alterations in the PSII electron transport and non-radiative loss of excitation energy in both photosystems. With the scope to gain further insights into the electro-optical interactions of CNTs with light-dependent photosynthetic reactions we used isolated photosynthetic complex (PSCs) with different level of complexity, such as thylakoid membranes, PSII-enriched membrane fragments and light-harvesting complexes of PSII. The energy and electron fluxes in the bio hybrid (PSCs/CNTs) systems were analysed by steady-state chlorophyll fluorescence and time-resolved fluorescence spectroscopy. The possible processes involved in the energy excitation decay in the photosynthetic structures in the studded model systems will be discussed.

Biography

Maya Dimova Lambreva has a PhD in Plant Physiology from Bulgarian Academy of Sciences. Since 2007 she is a researcher at the National Research Council of Italy. Her work is focused on the biophysical and biochemical aspects of the light photosynthetic reactions in microalgae and plants with the goal of developing bio-based applications employing photosynthetic organisms or photosynthetic elements. She has extensive expertise in different methods of chlorophyll fluorescence spectroscopy and in the quantification of photosynthetic activity. She has studied the correlation between structure and functionality of pigment-protein complexes involved in light transduction and conversion reactions of photosynthesis, using mutants of the model green algae *Chlamydomonas reinhardtii.* Currently, she is interested in using carbon-based nanomaterials for promoting the solar energy conversion in bio hybrid systems based on photosynthetic specimens.

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Ni-based catalysts for CO_2 conversion into CH_4: Advances in catalysts design and promotion effects

Leonarda F. Liotta
National Research Council (CNR), Italy

Global emissions of greenhouse gases, as CH_4 and CO_2, have been increasing in the last few decades and are recognized as one of the main anthropic causes of global warming. In this context, the Paris Agreement (ratified in 2016) sets the aim to hold the global warming well below 2°C. Many studies are focusing on CO_2 storage and chemical recycling. Among these methods, CO_2 methanation, also called Sabatier's reaction ($CO_2 + 4H_2 = CH_4 + 2H_2O$), is regarded as the most potential way for CO_2 utilization because of its high activity and moderate reaction condition, making it possible for commercial production. On the other hand, the so-called dry reforming reaction converting methane and $CO_2$to synthesis gas (DRM: $CO_2 + CH_4 \rightleftharpoons 2\ CO + 2\ H_2$) is another important reaction for getting value-added products from such greenhouse gases. The CO_2 methanation reaction is exothermic and thermodynamically favoured at low temperatures and high pressures, but when the reaction is carried out at temperatures typically above 300°C, the equilibrium increasingly favours several competing reactions, including the reverse water gas shift reaction, the Bosh reaction and the dry reforming of methane. Being all such side reactions exothermic, especially, the DRM reaction, high operating temperatures, usually in the range of 900–1273 K, are requested to achieve the desirable conversion levels.

Nickel catalysts are the most commonly used in CO_2 methanation and as well in the DRM. Reducible oxide supports and basic promoters enhance the reducibility of Ni catalysts, improve the CO_2 activation and boost carbon removal, thus, limiting the deactivation of catalysts occurring during DRM. Based on recent results on Ni catalysts for DRM and CO_2 methanation reactions, the present contribution will focus on an overview of catalyst design and promotion effects, focusing on the chemical composition and support effect in enhancing the catalytic performances.

Biography

Leonarda Francesca Liotta is Director of Research at the CNR-Institute for the Study of Nanostructured Materials (ISMN) in Palermo, Italy, and she works in the team Materials and technologies for environmental sustainability and energy efficiency. She has several international collaborations with distinguished scientists, among them: Prof. Olga Vodyankina, Tomsk State University, Russia, Prof. Patrick Da Costa, Sorbonne University, Paris, Prof. Anne Giroir-Fendler, University Claude Bernard Lyon 1, Prof Jean FrançoisLamonier, University of Lille, Prof. Renaud Cousin, University of Dunkirk, France, Prof. LyubaIlieva and Tatyana Tabakova of Bulgarian Academy of Sciences in Sofia.

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Direct laser patterning of photoluminescent semicondutor quantum dots in polymeric films

F. Antolini, R. Carcione and **F. Limosani**
ENEA Frascati Research Center, Italy

The aim of this work is to present the synthesis and some of the optical properties of the photoluminescent semiconductor quantum dots (QDs) obtained through the Direct Laser Patterning (DLP) technique in a polymeric film.

This study begins with the examination of the optical properties of the semiconductor quantum dots obtained by thermal decomposition of suitable precursors within the polymeric matrix. A this stage the effect of the different type of precursors and the presence of the ligands is discussed on the basis of the absorption and photoluminescent spectra.

The obtained luminescent nanocomposites are then characterised by absorption spectroscopy, photoluminescent spectroscopy and fluorescent microscopy. The results show that the laser patterning can be a suitable method for the generation of the semiconductor QDs in selected areas of the polymer. These results pave the way to exploit this technique in displays technology and are one of the main goals of MILEDI project.

Biography

Francesco Antolini is graduated in Chemistry and held is Ph.D in Biophysics on protein thin film technology and surfaces modification. Since 2000 he worked in the field of Material Science studying in the research area of nanostructured material synthesis and thin films technology. In the last years in the ENEA Agency he is involved in the chemical synthesis and photo-physical characterisation of nanostructured materials for lighting and sustainable development purposes. He has coordinated two EU projects in the field of nanomaterials synthesis and photonics.

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Microneedles fabrication technology for sensing and therapeutic applications

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Biosensing systems based on microneedles can overcome the stratum corneum of the skin, i. e. the outer natural barrier of the human body, without any pain and detect the target analytes directly in the interstitial fluid. Moreover, microneedle-based devices (MNDs) can combine diagnostic sensing and therapeutic administration of drugs in one single tool. From this point of view, more than a painless door to the human body, a MND represents the a perfect example of theranostic instrument, since a single device could quantify the real value of a relevant biomolecule, such asglucose, and accurately deliver a drug, the insulin, if needed. MNDs could be integrated on printed circuit boards, flexible electronics and microfluidic channels, thus allowing a continuous monitoring of the physiological parameters with very low invasiveness, together with sustained and localized administration of drugs. In fact, the transdermal route for drug administration is a very fascinating way, not only for the very low invasiveness and the easiness of self-administration, but also for the absence of first pass metabolism. However, the intercellular lipid matrix of the epidermis consists of ceramides, free fatty acids, and cholesterol, a complex mixture of neutral lipids arranged as bilayers with hydrophobic chains facing each other (lipophilic bimolecular leaflet). Transdermal delivery works only for lipophilic uncharged drugs with low MW (<500 Da), which needs low dose and continuous delivery. MNs can be used with both lipophilic and hydrophilic formulations, both charged and uncharged drugs, both small and oversized molecules.

For all these cases, MN configurations are illustrated, where the possibility to use solving or hybrid soluble/insoluble MNs are considered. MNDs can be designed for very specific applications, from the detection of skin cancer to the monitoring of metabolic pathways. Moreover, several fabrication approaches have been introduced, from laboratories to large-scale production.

Biography

Principia Dardanois responsible for the design, fabrication and optical characterization of optoelectronic silicon devices. She received his Ph.D. in Fundamental and Applied Physics at the same university in January 2008, with thesis on negative refractive index 2D photonic crystals in silicon. She is working at the Institute of Applied Science and Intelligent Systems (ISASI-CNR) in Naples, where she is the head of the photolithographic laboratory since 2006. She holds treeUS patent, and one Italian patent.

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High performance lithium silicide electrode enable by molecular layer deposition

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Silicon (Si) has become one of the most investigated materials for LIB negative electrodes because of its ability to accommodate 3.75 moles of Li per mole of Si ($Li_{15}Si_4$), leading to a theoretical capacity of 3,579 mA h g^{-1} at room temperature[1]. While 372 mA h g^{-1} is the theoretical capacity for graphite, the material used as negative in the current Lithium Ion Battereis. Despite Si advantages, progress towards a commercially available Si negative electrode has been impeded by their rapid capacity fade, poor rate capability, and low coulombic efficiency. The cause of electrode degradation is the Si volume change of ~300% upon lithium insertion and extraction, presenting a major problem for electrochemical performance.

One of the leading strategies established for the realization of such an approach is coating nano-Si particles with flexible materials to attempt to accommodate the volumetric changes of the particles. In this context, we propose to carry out a surface modification, in which Atomic Layer Deposition (ALD) and Molecular Layer Deposition (MLD) is utilized to grow a mechanically robust, flexible coating, to undertake the Si expansion and contraction. the recipe here developed is based on Glycerol and $TiCl_4$ as the titanium precursor.

The composition of the films was studied using Fourier-Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscope-Energy-dispersive X-ray spectroscopy (SEM-EDX). Cyclic Voltammetry was used to characterize the electrochemical performance of the LixSi negative electrode coated with titanicone. We have successfully shown the deposition of titanicone on LixSi electrode and an initial electrochemical assessment of this electrode. Typical voltammogram shows the formation of the solid electrolyte interface, evident in the first cycle. In the subsequent scans, these peaks disappear. The sample exhibit the regular waves are corresponding to the Si redox reaction.

Biography

Zahilia Caban Huertas (Ph.D. chemistry) now a Marie Currie Fellow at Aalto University. She got her B.Sc. in chemistry at the University of Puerto Rico Rio Piedras Campus, during this time she was awarded with the Puerto Rico NASA Space Grant Consortium Scholarship. She stars her adventure in scientific research working with Fuel Cells in Puerto Rico. She got her M.Sc. and Ph.D. at Autonomous University of Barcelona. Her doctoral research was focus in the development new approaches to fabricate LiFePO4 electrodes, this work was done at the Catalan Institute of Nanoscience and Nanotechnology. Her more resent interest are Lithium Solid State Batteries and Solid State Electrolytes.

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An efficient four-variable I-L nonlocal dynamic model of unsymmetrical plane sandwich structure with laminated facings – Acoustic application

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Warsaw University of Technology, Poland

This presentation is devoted to a new, simple, containing only four unknown functions, individual-layer, dynamic model for bidirectional sandwich structure (plate) and unidirectional sandwich structure (strip) which are unsymmetrical with respect to their middle planes. The shear strains in the outer layers of the structures are neglected while the shear strains in the middle layers are variable and equivalent to zero on their outer surfaces. Local constitutive models of the layers consistent with the assumed kinematics are derived. A detailed analysis of all partial problems is presented. In order to determine the unknown functions, appearing in the kinematic models assumed, one needs to solve a set of three coupled partial differential equations and separately a fourth governing equation that contains only one unknown function. In the case of the structures symmetrical about the middle plane only two uncoupled partial differential equations must be solved. The application of this model for determining the acoustic resistance (transmission loss) of the structure considered for the plane acoustic wave is shown.

Biography

Stanisław Karczmarzyk is employed as an assistant professor at the Faculty of Automotive and Construction Machinery Engineering of the Warsaw University of Technology. Since 2015, he has conducted two original lectures: (1) Computer modeling in engineering practice and (2) Non-local and local computational models of acoustic resistance of layer structures. For both of these lectures he wrote original, reviewed scripts for students, published by the publishing house (OWPW) of the Warsaw University of Technology.

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Microstructure dependent corrosion of Mg-Li alloys

A. Dobkowska and **J. Mizera**
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Increasing pressures associated with environmental factors such as carbon oxides in the atmosphere and increasing fuel costs are driving many industrial branches to look for advanced lightweight materials with the lowest possible densities such as magnesium or aluminum alloys. One way to decrease the weight of the materials is the use of alloying elements such as Li, which has a density of 0.534 g cm^{-3}. Li can reduce magnesium alloys densities from 1.75 g cm^{-3} for the AZ31 alloy and its addition improves their mechanical properties.

This study describes the corrosion resistance of dual-phased Mg-7.5Li-3Al-1Zn (AZ31+7.5Li). The microstructure of the extruded conventionally, and the extruded by forward-backward extrusion with a rotating die (KoBO) was characterized using scanning electron microscopy (SEM) in backscattered electron mode (BSE), and by electron back scattered diffraction (EBSD). The X-ray diffraction (XRD) was made to recognize phases formed in the materials. The alloys microstructures consisted of α (Mg), β (Li), $MgLi_2Al$ and $Mg_{17}Al_{12}$. The potential under open circuit conditions, potentiodynamic and mass loss measurements in chloride containing solutions were done to describe the corrosion behaviour of the alloys.

The results showed that corrosion of dual-phased Mg-Li alloys is microstructure dependent, and is related to the relative concentration and distribution of β(Li) phase in the α(Mg) matrix. In the traditionally extruded alloys, the higher amount of β (Li) reduces the area ratio of cathodic to anodic sites of corrosion. The corrosion behaviour of the materials extruded via KoBo was varied due to different distribution of β (Li) phase in the α (Mg) matrix.

Biography

Anna Dobkowska is a specialist in the microstructure dependent corrosion of light alloys and copper based materials. She defended her PhD in 2017 at The Warsaw University of Technology in Poland. From 2018 to 2020 she worked with Electrochemistry Group led by prof. David Shöesmith and prof. Jamie Noël at The Chemistry Department, The Western University of Ontario in Canada. Since she has been working on the project sponsored by The Nuclear Waste Management Organization (Toronto, Canada) to determine the effect of substrate impurities on copper corrosion behavior. This project was related to the long-term management of used nuclear fuel in Canada. The experience gained during her stay at The Western University of Ontario and her previous experience at The Warsaw University of Technology has enabled her to become a materials science specialist with significant expertise in corrosion, electrochemistry, and surface analytical and materials characterization techniques.

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Monitoring the effect of amino acid on the corrosion process of metal based on comprehensive micro- and nanospectroscopy investigations

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Corrosion is a very serious global problem in the various branches of industry. Metals are constantly exposed to the natural environment and aggressive media, thus there is a need to protect them from corrosion. One of the most effective strategies for improving corrosion resistivity of metallic materials is surface modification.

The main goal of our research is to study the influence of surface modifications of metal materials using potential inhibitors such as amino acids and nanoparticles (NPs) on the corrosion resistance of these materials and to investigate phenomena that occur at the metal/potential inhibitor interface. The use of organic inhibitors, such as amino acids, has many advantages. Amino acids have been used in various applications for many years. Modification of metallic surfaces, such as the interposition of nanoparticles into metal materials, is one of the methods which can provide corrosion resistance.

In thestudies of the corrosion inhibition process by the above-mentioned compounds, we applied mainly: spectroscopic methods such as Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy (RS), and techniques based on the surface-enhanced effects such as surface-enhanced infrared absorption spectroscopy (SEIRA), surface-enhanced Raman spectroscopy (SERS). Moreover, the technique which combined conventional IR with atomic force microscopy resulted in a nano-SEIRA technique was used. These methods are great tools for studying corrosion products structure, their distribution on the corroded surface, as well as adsorption processes of potential bio-inhibitors. The application of SERS and SEIRA techniques gives a detailed description of the adsorption of threonine onto the iron surface. Threonine influenced the process of corrosion of the investigated surface due to the existing strong interaction between the protonated amine and carboxylate groups and CuNPs deposited onto the iron surface. The obtained results confirmed that there is a good correlation between the spectra recorded by the SERS, SEIRA, and nano-SEIRA techniques.

Biography

Dominika Święch is an Assistant Professor at the AGH University of Science and Technology in Krakow (Poland). She obtained her PhD degree in chemistry (molecular spectroscopy) at the Faculty of Chemistry, Jagiellonian University in 2014. She was Research Fellow (2013) in the lab of Prof. Yukihiro Ozaki (School of Science and Technology, Kwansei-Gakuin University, Japan). In 2018, shewas working at the Institute of Nuclear Physics Polish Academy of Sciences in Krakow (Poland) during a research internship.Her present research topic is the study ofthe influence of surface modification of metallic materials by potential inhibitors (amino acids and nanoparticles) on the corrosion resistance of these materials and to investigate phenomena that occur at the metal/potential inhibitor interface (Principal Investigator, project titled "Spectroscopic studies in micro- and nanoscale of the corrosion process and its inhibition of the modified metallic surfaces applied in implantology" founded by National Science Centre, Poland, No. 2019/35/D/ST4/02703).

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W-Zr-B coatings deposited by RF Magnetron – PLD hybrid method

R. Psiuk, D. Jarząbek, P. Denis and **T. Mościcki**
Polish Academy of Sciences, Poland

Transition metal borides even in the form of thin films exhibit unique combinations of properties such as high melting points (TiB_2, ZrB_2 T_m>3400K), high hardness (ReB_2, WB_4 H>40 GPa), high thermal and chemical stability, and excellent corrosion and oxidation resistances, that is why in recent years they arouse interest in the research community. In this work, (W, Zr) B_2 films with the different stoichiometric ratio Zr/W deposited by RF magnetron sputtering and hybrid PLD-RFMS methods are presented. Zirconium amount in coatings was increased by increasing the laser power (fluence) on ZrB_2 rotating target. $WB_{2.5}$ target was magnetron sputtered with constant power. The results show the possibility of controlling of phase composition, structure and utility properties of thin films made of novel super-hard tungsten borides doped by Zirconium. In the case of (W,Zr) Bx, this technique enables also precise control of the doping process. Coatings were tested by means of SEM, EDS, XRD, nanoindentation and micropillar compression. The deposited pure WB_2 coatings have crystalline columnar structure with an average feature size of 23 nm and 001 preferred orientation. The columns are separated by a thin, 1-2 monolayers B-rich amorphous phase what guaranteed hardness H= 48.9±0.6 GPa. Different amounts of zirconium can affect phase composition and crystallinity of the coatings. High preserved hardness (up to 50 GPa) and values of elastic recovery higher than 60% suggests that they may be more resistant to cracking than pure WB_2 coatings. Increased fracture toughness with preserved high hardness shows that solid solution strengthening is a good method to enhance the properties of tungsten diboride coatings.

Biography

A graduate of the Faculty of Materials Science and Engineering of the Warsaw University of Technology. In his engineering and master's thesis he dealt successively with PPS pulse plasma sintering and 3D printing using the SLM method. Currently an employee and doctoral student at the Institute of Fundamental Technological Research of the PAS. The subject of the PhD thesis is super-hard layers of tungsten borides with zirconium addition by magnetron sputtering and/or laser ablation.

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Photoluminescence of carbon nanoparticles synthesized by laser ablation in water and aqueous solutions of amine-based reagents

A.Kaczmarek, J.Hoffman, P.Denis and **T.Mościcki**

Polish Academy of Sciences, Poland

The comparison between two synthesis routes for obtaining carbon nanoparticles (CNPs) in water and in aqueous solutions of amine-based reagents is presented. The influence of synthesis approach and parameters on structural and luminescent properties of CNPs is discussed.

Each of the synthesis routes was a two-step process. In the first approach, the graphite target submerged in water was ablated using moderate fluence of a laser beam. Next, a certain amount of aqueous reagent solution was added to the suspension of carbon particles. Such a mixture was then exposed to a much stronger laser beam in order to reduce the size of particles. In contrast to the first approach, during another synthesis route the graphite target was immersed in aqueous reagent solution and exposed to laser irradiation. The obtained suspension of carbon nanoparticles was further irradiated without the presence of graphite target.

Luminescence and absorbance studies revealed interesting properties of obtained colloids. Suspension of particles produced in pure water after first step is yellowish and has some absorbance in whole spectrum rising as the wavelength decreases. After second step it is colourless and fully transparent in visible light and has high absorbance in UV with distinct maximum about 285 nm. The addition of the reagent at the second step of the synthesis leads to location of absorbance maximum at about 285 nm. However, using amine-based solution from the beginning causes high absorbance in the whole spectrum without any distinctive maximum. It may indicate the simultaneous creation of different carbon structures and fluorescent molecules during laser ablation process.

Biography

Agata Kaczmarek is a PhD student and a young researcher in the Institute of Fundamental Technological Research PAS (Poland). She works in the field of nanotechnology and materials science. Her main area of interest is nanoparticles synthesis by means of Pulsed Laser Ablation in Liquids (PLAL). She graduated in Nanotechnology at Gdansk University of Science (Poland). After graduation; she gained experience in additive manufacturing while working in XTPL S.A. In this company, she was holding a position of R&D engineer in applications laboratory and was responsible for ultra-precise deposition of materials, mainly inks with nanoparticles.

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Analysing the impact of hydrophobic coatings on the reduction in soil accumulation on transparent surfaces intended for PV application

M. Rudnicka and **E. Klugmann-Radziemska**
Gdańsk University of Technology, Poland

Energy yield possible to obtain from photovoltaic (PV) installation is directly correlated to current weather conditions and the state of individual modules. The latter may be compromised by any residue deposited on top of the glass coverage. Dust settlement causes reduction of working parameters, which in turn leads to lesser amount of light irradiation reaching PV cells. The rate of soil accumulation is linked to exact location of solar installation, type of pollution, any heavy industry in the area and module tilt angle. Some areas are impacted with much more prominent dust deposition, which covers the module surface faster and therefore calls for the increase in manual cleaning.

An approach to mitigate this effect is adding transparent hydrophobic layer on the front glass cover. An analysis of few materials available on the market was carried out to test their possible application in PV industry. One important information that was observed immidiately after performing irradiation test was that any glass coverage leads to transparency reduction. This happens notwithstanding the fact if the glass plate was enhanced with hydrophobic film or without it. Furthermore, a slight negative impact of few percentile points is caused by the hydrophobic film itself. Therefore, it is most important to fabricate such layer that does not cause any additional transparency reduction. Subsequent test study with different type of dust helped to conclude that the analysed coatings may indeed pose a good candidate for the use on PV modules. It should be mentioned that they may be improved in further studies, as the authors would like to enhance their transparency.

Biography

Małgorzata Rudnicka in 2018 received MSc degree in technical physics at Gdańsk University of Technology (GUT), Poland. For the time being she is a PhD student at the Department of Energy Conversion and Storage, Faculty of Chemistry, GUT. The current field of interests revolve around photovoltaics and soiling effect occurring on the surface of solar modules.

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The effect of plasma treatment of polyethylene powder on the mechanical properties of composites prepared by rotational molding

Z. Ghanem, H.Šourková ,T. Vacková, P.Špatenka, Z. Jeníková, J. Sezemský and **J. Antoň**
Czech Technical university, Czech Republic

Rotational molding, as well as 3D printing technologies, is based on sintering of raw materials under the ambient conditions. No additive pressure can be added to form a good adhesion between the matrix and the filler. Due to these conditions, the mechanical anchoring of the matrix to the filler that dominates the injection molding is not the case, and the formation of chemical bonding is necessary for good wetting and strong adhesion.

Cold plasma surface treatment has been established as an effective and low-cost technology for surface hydrophilization of polymer materials without altering properties of bulk material. In our research untreated polyethylene (PE) and plasma modified polyethylene (PPE) as a matrix for composites produced by rotational molding has been studied as a model for non-pressure technologies Short glass fibers at different percentage were manually mixed with untreated and treated linear low density polyethylene powder and used to prepare a samples using laboratory scale rotational moulding machine. A new approach of using polyethylene waxes as a sizing agent was introduced. The scanning electron microscopic images showed that the addition of plasma treated polyethylene waxes improved the adhesion between the glass fibres and plasma treated polyethylene. Mechanical tests also showed an improvement in tensile and flexural modulus of the composites prepared by treated materials.

Biography

Zoya Ghanem holds a bachelor's degree in mechanical engineering from Tishreen University in Latakia-Syria and a master's degree in manufacturing and material engineering from Czech Technical University in Prague. She is currently a PhD student and a researcher at Czech Technical University in Prague in the Department of material engineering. She researches in the field of thermoplastic composites including preparing samples and testing them and analyzing the data, moreover, she gives lectures, writes research papers, reports, reviews and summaries.

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Ensuring electrical conductivity of polymer-based component

J. Antoň, P. Špatenka and **L. Cvrček**
Czech Technical University, Czech Republic

The poster deals with a topic of electrically conductive plastics and polymers. Based on the conduction parameter PE-HD filled with carbon was selected for our investigation. Mechanical properties and material composition were analyzed by tensile strength, Charpy impact test and SEM. Low value of toughness was observed probably due to low adhesion between the PE matrix and the carbon filler and the glass fibres reinforcement.

Plate formed sample was contacted by Al and/or Cu electrodes. Using various methods including galvanic plating, cold spray deposition and physical vapour deposition (PVD).

A criterion based on a climatic test with a rapid temperature change (IEC 60068-2-14) was introduced to evaluate the quality of the adhesion of the coating to the surface of the part. The best result had the coating created by Physical Vapour Deposition technology. This coating was also subjected to an increased number of temperature changes and a more demanding cold environment (from -196°C to 100°C) and even in this case the adhesion of the coating to the substrate was not damaged. The material itself was tested for electrical conductivity and calorific value by electric current. The conductivity of the material is in the order of 10^{0} – 10^{-1} S/cm.

Biography

Jakub Antoň has obtained the master's degree in design and manufacture of plastic and composite components at the Czech Technical University in Prague. In his diploma thesis he dealt with the issue of conductive plastics. Now he is a postgraduate student at the CTU at Department of Materials Engineering. He has been working in materials science for several years. He focuses mainly on 3D printing of composite materials and conductive plastics.

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Solid materials as green catalysts for bioenergy processes: A review as a sustainable perspective

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[2]Instituto Superior Técnico, Portugal

The purpose of this presentation is to highlight several chemical applications to produce, mainly, bioenergy and new major-value products, under new materials, as potential heterogeneous green catalysts. Some of these applications were tested in lab, under different chemical and electrochemical processes. The increase on its utilization of new chemicals as potential heterogeneous catalysts for bioenergy processes, is increasing significantly since last years, performing a remarkable attention with these materials, as an important tool for the application of the green chemistry concept. Composite materials, nanocatalysts, zeolites, double oxides, natural clays and other natural/ synthetic materials are commonly used as sustainable solid catalysts in bioenergy processes, e. g., in 1st and 2nd G biodiesel processes (acid and alkaline catalysis) and, in syngas conversion processes combined with hydrogen technologies (methanation reaction, production of methanol, DME, phormaldeyde, formic acid, etc.). Glycerol valorisation processes will be, also exemplified, as sustainable ones with the utilization of these materials as potential heterogeneous catalysts, in acetalization and acetylation reactions, to produce new major value products, such as, biofuel additives in diesel engines. Heterogeneous catalysis presents several and significative processual advantages when compared with the heterogeneous ones, regarding not only, economic advantages, but also, regarding the minimization of environmental impacts, key factors for applying any sustainable process, at industrial scale. Heterogeneous catalysis is a major and crucial factor to addressed sustainability, as one of the precursors of green chemistry in industrial process, combining science materials, physics, chemistry, and chemical engineering profiles, thus enhancing the utilization of multidisciplinary teams.

Regarding, for instance, biodiesel production process, the utilization of some of these materials produced a biofuel with higher conversion and yield, higher than 96.5% (w/w), which is the minimum required by EN 14214 European Standards for biodiesel quality.

Biography

Jaime F. B. Puna has completed his PhD in 2014, at Instituto Superior Técnico, University of Lisbon, regarding biodiesel production under heterogeneous catalysis. He is Adjunct Professor at ISEL, in the Chemical Engineering Department, with more than 20 years of experience. The research interests are addressed to the fields of bioenergy, waste valorisation, biofuels, heterogeneous catalysis, and nano materials. He is responsible for the Chemical Technology Lab at ISEL. He was PI researcher of I&DT projects related with biofuels and green heterogeneous catalysts.

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Theme: Navigating the future research directions in the field of Materials Science and Engineering

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Functionally-graded materials and complex alloy systems through WIRE-ARC additive manufacturing

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Wire-arc additive manufacturing (WAAM) is receiving increasing attention due to advantages in terms of component costs, deposition rate and buy-to-fly ratio of structures of medium-to-large complexity. The use of multiple alloy wires during WAAM is of particular interest as the chemical composition of the deposit can be adjusted according to the structure's requirements without the limitation of commercially available welding wires. Additionally, the local chemical compositions may be adjusted yielding novel physical and mechanical properties of such functionally graded materials (FGM).

The present work explores options for the fabrication of structures using multiple feedstock wires to a deposit a FGM and b deposit alloy compositions of commercially unavailable materials. For the deposition gas tungsten arc welding (GTAW) is used. Resultant materials are characterized regarding chemical composition, microstructure and mechanical properties. Utilizing tailored processing conditions the fabrication of a chemical gradient was verified by optical emission spectroscopy along the specimen height with the results for Si. The major findings of the presented research can be concluded as follows: WAAM using two feedstock wires is not only feasible but allows for flexibility in the processing routine; The adjustment of new alloy compositions by mixing the respective feedstock wires in situ during processing is possible with sufficient intermixing; Microstructures and resultant properties can thereby be adjusted locally; The outcomes of this work expand the applicability of WAAM as additional design freedom is gained for the fabrication of structures and components.

Biography

Thomas Klein studied Materials Science at the Montanuniverstät Leoben, Austria, where he received his Masters degree in 2013 and his PhD in 2017 for the characterization of phase transformations, microstructure formation and mechanical properties of inter metallic alloys based on TiAl. After a Post Doc assignment at the Materials Center Leoben (MCL), Austria, from 2017 - 2019, where he focused on the development of advanced high strength steels, Thomas Klein joined the LKR Light Metals Technologies Ranshofen working on the development of novel light-metal alloy system for wire-arc additive manufacturing.

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Electron concept for hydrogen brittleness of metals

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The reversible or "true" hydrogen embrittlement, HE, is related with movement of dislocations accompanied by hydrogen migration and, for this reason, manifests itself in a certain range of temperatures and strain rates, where hydrogen atoms can follow dislocations.

The proposed concept attributes HE to hydrogen effect on the weakening of interatomic bonds within hydrogen atmospheres around the dislocations, which locally affects the shear modulus μ and, consequently, decreases the start stress of dislocation sources, $\tau \approx 2\mu b/L$, where L is a distance between pinning points, diminishes the line tension of dislocations, $\Upsilon \approx (\mu b2/4\pi)/\log(\Re/5b)$, where $\Re$ is the radius of the dislocation curvature, which enhances mobility of dislocations, and reduces a distance between dislocations in their plane assembles, $d \approx (\pi\mu b)/16(1-\nu)n\tau$, where τ is the shear stress in the slip plane, which increase the number of dislocations, n, in the pileups and, correspondingly, the stress at a leading dislocation $\tau_L = n\tau$.

This concept is substantiated by the ab initio calculated hydrogen-decreased density of electron states at the Fermi level in Fe-, Ni- and Ti-based alloys, corresponding increase in the concentration of free electrons measured using the electron spin resonance and studies of hydrogen effect on dislocation properties by means of mechanical spectroscopy.

Biography

Valentin Gavriljuk student of Kiev Technical University, speciality in physical metallurgy, 1955-1960. Engineer, head of technological bureau at mechanical engineering factory, Minsk, 1960-1962. Postgraduate at Institute for Metal Physics, IMP, in Kiev, PhD in Metal Physics, 1962-1965. Senior scientific researcher, doctor hability, professor of solid state physics, IMP, 1966-1988. Head of department of physical principles for design of steels and alloys, IMP,1989-2015). Principal scientific researcher, IMP, since 2016. Professor at Kiev branch of Moscow Physical-Technical Institute (2002-2016). Currently, he is a Professor of Kiev Academic University (since 2016).

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Preparation, investigation and widespread utilization of bacterial cellulose-ZnO-MWCNT hybrid membranes

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University of Miskolc, Hungary

Self-supported and flexible bacterial cellulose (BC) based hybrid membranes were synthesized and decorated with zinc oxide/multi-walled carbon nanotube (ZnO-MWCNT) composite additives in order to modify and tune their surface and bulk properties. Two types of ZnO-MWCNT additives with different morphologies were used in a wide concentration range from 0 to 90% for BC-based hybrids produced by filtration. The novel photoactive membranes have grabbed the attention in the field of environmental protection by employing wastewater treatments and the removal of microorganisms or organic pollutants from wastewater. Here we present a promising self-supported photoactive hybrid membrane for future antimicrobial and water treatment applications. In this study, the efficiency of bacterial cellulose (BC) - zinc oxide (ZnO) - multi walled carbon nanotube (MWCNT) hybrid membranes in the adsorption and photocatalytic degradation of methylene blue (MB) under UV radiation and the removal of Escherichia coli (*E. Coli*) was investigated. It was found that the photocatalytic efficiency is strongly dependent on both the preparation method and the amount of ZnO-MWCNT additives loaded into the hybrid membranes. The characterization of BC-ZnO-MWCNT membranes was done using focus ion beam scanning electron microscopy (FIB-SEM), energy dispersive X-ray spectroscopy (EDS), X-ray powder diffraction (XRD), mercury intrusion porosimetry (MIP), X-ray micro computed tomography (μCT), dynamic light scattering (DLS), contact angle measurement, surface area measurement (BET) and Raman spectroscopy to study the morphological aspect of the prepared-membranes. The promising results of this study could provide a new pathway in the field of photocatalysed-based water treatment technology by the application of hybrid membranes.

Biography

Zoltan Nemeth obtained his PhD in 2014 from the University of Szeged, Hungary. In 2014 he got the opportunity from the SciEx Program Committee to attain his postdoctoral fellowship entitled Ceramic paper-based, highly efficient virus immobilization and inactivation, in Prof. Thomas Graule's research group at Empa, Switzerland. His main research topics are the development of hybrid nanostructures, hybrid materials and nanocomposites. He currently works at the Institute of Chemistry – University of Miskolc as a senior research fellow.

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Synthesis of $ZnTiO_3/TiO_2$ nanocomposite supporting in Ecuadorian clays for the adsorption and photocatalytic degradation of methylene blue

Ximena Jaramillo-Fierro[1,2], Silvia González[2], Hipatia Alvarado[2] and **Francesc Medina[1]**

[1]*Universitat Rovira i Virgili, Spain*
[2]*Universidad Técnica Particular de Loja, Ecuador*

Semiconductor research has shown great promise in recent times in photocatalytic remediation of harmful organics from air and water. A variety of semiconductors has been explored in this modern photoassisted techniques, including metal oxides such as TiO_2, ZnO and their derivate. In the present study $ZnTiO_3/TiO_2$ was prepared by sol-gel method using Zn $(CH_3COO)_2$-$2H_2O$ and $Ti(OC_3H_7)_4$ as reagents. The effect of several conditions such as reaction temperature and TiO_2: ZnO proportion on morphology and purity of products was investigated, and the optimum conditions for the synthesis of photocatalysts were found. A systematic study on the structural, morphological and photocatalytic properties of $ZnTiO_3/TiO_2$ was carried out using various techniques. SEM images reveal that the $ZnTiO_3/TiO_2$ has a typical particle size of about 100 nm with quasi-spherical shape. The adsorption and photocatalytic activity was investigated by discoloration of Methylene Blue (MB) as an organic pollutant under UV irradiation in both, TiO_2 and $ZnTiO_3/TiO_2$ supported over some Ecuadorian clays. The materials evaluated were prepared in the form of 1.0 cm long and 0.2 cm in diameter cylindrical extrudates. The degradation percentage of MB obtained was 85% approximately after 150 min of irradiation. The obtained results allow us to conclude that these synthesized materials can be used as adsorbents and photocatalysts.

Biography

Chemical Engineer and Master of Applied Chemistry (Universidad Técnica Particular de Loja - UTPL, Loja-Ecuador). Ph.D. candidate in Nanoscience, Materials and Chemical Engineering (Universitat Rovira i Virgili, Tarragona-Spain). Experience in molecular modelingand synthesis and characterization of materials with different technological and industrial applications. Director of undergraduate and master's thesis at UTPL. Professor at UTPL in careers related to Engineering and Chemistry, teaching the following subjects: Development and Application of Catalysts, Chemical Kinetics and Engineering of Chemical Reactions, Thermodynamics, Heat Transfer, Industrial Processes, Solid State Chemistry and Crystallography, Inorganic Chemistry, Biochemistry, Applied Physics, Polymer and Petroleum Technology, Ceramics and Cement Technology. Currently coordinator of the New Materials Laboratory at UTPL.

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Microstructure conditioning in an advanced boron-containing complex phase steel heat treated within the Q&P process concept

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[2]*TechnologicalInstitute of Saltillo (ITS), Mexico*

Emerging ferrous alloys are part of a recent group of newer and promising high-performance engineering materials. The development of novel alloy design and physical structure reflects the interest in improving the flexibility of material treatment in its production stages due phases' constitution and transformation over microstructure evolution. In this way, the development and implementation of advanced high-strength steels (AHSS) represent being the best solution to meet high levels of safety and environmental care, demanded to the automotive industry. The objective of this research work is to evaluate the effect of quenching temperature above and below the martensitic start line transformation (Ms) on the microstructure evolution of a complex phase steel, belonging to the 3rd generation AHSS, micro-alloyed with boron when it is heat treated based on the Q&P process concept of one and two steps. For this purpose, an experimental single micro-alloyed with boron (60 ppm) complex phase steel was fabricated and hot and cold rolled. After that, the steel was homogenized and quenched in a salt bath at 420 and 380°C, respectively. Then, the steel was tempered following one-step (isothermally condition) and two-steps (reheated at 600°C) process, respectively, for carrying out the partition process. Finally, structural, microstructural and mechanical characterization was carried out with the aim to determine steel microstructure conditioning. In general terms, outstanding results have been obtained regarding to the austenitic grain size refinement after the Q&P heat treatment. Microconstituents such as retained austenite, martensite, bainite, ferrite and some perlite were obtained, homogeneously distributed in the two-steps Q&P steel microalloyed with boron and quenched at 420°C. Furthermore, high values of mechanical resistance superior to 1300 MPa were obtained. All this when compared with the obtained results in the remaining studied conditions for the non-microalloyed and boron-containing complex phase steel.

Biography

Antonio Enrique Salas Reyes born in 1983, Mexico. He studied ferrous metallurgy and holds a M.Sc. in metallurgical engineering from the Technological Institute of Morelia. In December 2014, he received his Ph.D. in metallurgy and materials science from University of Michoacan (UMSNH)-Mexico. During his Ph.D. studies, he realized a research stay abroad in the Polytechnic University of Catalonia, Barcelona, Spain. He has worked in specialized steel industry companies such as TenarisTamsa and Imexaza (belonging to Imesaza-Spain) in Mexico. He is currently a Full Time Professor in the Department of Metallurgical Engineering of the Faculty of Chemistry of the National Autonomous University of Mexico (UNAM) in Mexico City.

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Effect of cooling rate and alloying elements on Al-Si-Fe alloys

I. A. Figueroa and **V. A. Aranda**
National Autonomous University of Mexico(UNAM), México

The microstructural and mechanical analysis of a ternary Al-20Si-5Fe (wt%) system with Cr Mn, and Ti additions are presented and discussed. The manufactured alloys were characterized by means of XRF, XRD, SEM, TEM as well as Vickers microhardness and compression tests. For the master alloy, the microstructural analysis revealed the presence of Al phases, eutectic silicon (SiE) and primary silicon (SiP). When adding the alloy elements, the presence of Al_3FeSi_2 was observed for all systems. When the addition of transition elements increased in a proportion of 1, 3 and 5 wt%, respectively, the presence of the intermetallic $Al_{95}Fe_4Cr$, Fe_4MnSi_3, $Al_{19}Fe_4Mn$, Ti_5Si_3 phases was observed. For the AlSiFe-Cr system, it was found that the acicular intermetallic Al_3FeSi_2 (2D) obtained by conventional solidification showed a plate-shaped structure (3D). The highest microhardness value was found for the alloys with 5 wt% of Cr (220 HV) in conventional solidification. However, for suction casting the highest microhardness was 192 HV (3 wt%). Although the microhardness decreased with the rapid solidification, the compressive plasticity of the alloy increased considerably (> 300%), being the microstructural homogeneity the main contributor to the ductility behavior. The AlSiFe-Ti system showed a homogeneous dispersion of the intermetallic Al_3FeSi_2 and Ti_5Si_3 phases as the amount of Ti increased. The presence of Ti_5Si_3 did favor the ductility, increasing by 200%, when compared to that of the master alloy. Finally, these results demonstrated that Ti enhanced the plastic deformation, whilst Mn improved the microhardness and toughness. The addition of Cr provided a good balance between plastic deformation and toughness.

Biography

Ignacio A Figueroa joined the Institute for Materials Research at the National Autonomous University of Mexico in 2010 from the Advanced Manufacturing Research Centre with Boeing -Rolls Royce Factory of the Future- in Sheffield (UK), where he was a Research Fellow. He obtained his PhD in Engineering Materials from the University of Sheffield (UK) in 2008. He has been awarded with level III of the National System of Researchers (the highest). Distinction in the field of "Technical Creativity or Invention", awarded by the foundation Mexico with Values (Mexico con Valores). The 2015 National Sustainable Energy Award by the Secretary of Energy and the World Energy Council. The National Autonomous University of Mexico-UNAM recognized with the National University Distinction for Young Academics 2016 in the area of "Technological Innovation and Industrial Design". In 2018, CONACYT awarded him with distinction of "Casos de Éxito" (Success Cases). Also in 2018, the Mexican Academy of Sciences awarded him with the 2018 RESEARCH PRIZE in "Engineering and Technology". Finally, in 2021, at the Webinar on Materials Science, Engineering and Technology, he received the "Vebleo Scientist Award" for his contribution to the progression of his research field.

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Increment of CO_2 adsorption capacity of nanostructured wool activated carbon fibers by nitrification

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[1]Universidad de la República, Uruguay
[2]Centre national de la recherche scientifique, France

The XXI century started with high defying environmental issues. Among them, global warming due to greenhouse effect is one of the most important regarding its impact and interest shown by the scientific community. Several gases emissions (mainly carbon dioxide and methane) had been identified as contributing factors to this situation. Various technologies had been developed in order to achieve CO_2 sequestration, being chemical and physical extraction the most used. Adsorption based technologies have gained ground in this matter and their use has become another important industrial option. The development of adsorbent materials with high CO_2 adsorption capacity is related with this methodology and it is the center of this work. Nitrogen presence in adsorbents has been associated with increase in CO_2 adsorption and, as wool is rich in nitrogen due to its proteic nature, it was chosen as a carbonaceous adsorbent precursor. Pristine fibers were submitted to air stabilization, carbonization and physical activation with CO_2. Key temperatures of the process were selected by thermal analyses in different atmospheres. In order to explore the role of nitrogen in the adsorption, additional nitrogen functions were incorporated by heating the stabilized wool in nitric/sulphuric acid solutions, using acid concentration as variable. CO_2 adsorption kinetics and isotherms were performed on modified and unmodified fibers and an increase on CO_2 adsorption was observed for higher adsorption pressures. Kinetics data adjust to a pseudo second order model in all cases. Composition changes were verified by elemental analysis and Infrared spectroscopy. Raman and XR analysis were used to obtain additional information about physico-chemical changes occurring during the different processes.

Biography

Alejandro Amayal is Dr. in Chemistry of Faculty ofChemistry (FQ), Universidad de la República (Udelar), Montevideo, Uruguay, 2011. He works as Professor of the Physical Chemical Area and Deputy Chief of The Renewable Energy Area in the Pando Technological Pole Institute. Professor in charge of the Chemistry Teaching Academic Unit (all in FQ, Udelar). His main fields of research are related to the obtention, characterization and use of carbonaceous materials in environment and energy fields. His primary interest is the add of value to agro-industrial residues rich in carbon by the production of carbonaceous materials of industrial interest. The main uses for these materials are remediation (adsorption of classical and emerging contaminants), gases mixtures separation and gas sequestration, and fuels (biomethane, hydrogen, torrefaction, pyrolysis, combustion).

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Direct synthesis and pH adjustment approaches to incorporate zirconium species in SBA-15 mesoporous silica

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[1]Universidad de Concepción, Chile
[2]Universidad de Los Andes, Venezuela
[3]Universidade do Porto, Portugal
[4]Universitat Politècnica de Catalunya, Spain
[5]Universitat Rovira i Virgili, Spain

A comparative study of synthetic procedures by hydrothermal treatments at 60°C for the preparation of a series of Zr-SBA-15 materials (Si/Zr=∞, 10, 5, and 2) using direct synthesis (method A) and pH adjustment (method B) approaches is reported. The method B uses concentrated ammonia as a pH regulator and a further hydrothermal treatment. It shows a decrease in the Si/Zr ratio measured by EDS and XPS as the Zr content increased in the preparation by both methods. XPS revealed lower values of Si/Zr ratio with respect to EDS, which suggests more content of surface zirconium species than bulk. All N2-physisorption isotherms show type IV behaviors which are characteristic of mesoporous materials. Regardless of the preparation method, the BET specific surface area (SBET) and pore volume (Vp) values show a decreasing trend as Si/Zr ratio decreases. The pore size (dp) indicates diameters below 4 nm, except in the SB sample.

Low-angle diffraction patterns show a peak associated with the (100) plane, which tends to widen and decrease in intensity for materials prepared with higher zirconium charges, revealing the presence of mesoporous structure. HRTEM corroborate the mesoporous arrangements of short- and long-range order, depending on the conditions. SEM-EDS mapping suggests a homogenous distribution between zirconium and silicon species over the SZA-10 and SZB-10 materials. It is concluded that the decrease of Si/Zr ratio modifies the structural, textural, and surface properties of the materials, and consequently, compromising the ordered arrangement of the mesopores. Finally, the pH adjustment method leads to better preservation of mesoporous order.

Biography

Julio Colmenares-Zerpa is currently a Ph.D. student under the supervision of Prof. Ricardo Chimentão at the University of Concepción in Concepción, Chile. He received his B.S. in Chemistry in 2017 from University of Los Andes in Mérida, Venezuela. He got a Ph.D. scholarship (N° 21201413) by the National Research and Development Agency of Chile. His doctoral research is focused on the preparation of catalytic materials for application in the valorization of glycerol for obtaining high-value chemical compounds.

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Extraction chromatography materials prepared with MIBK on amberlite®XAD4 and PTFE

F. Monroy Guzmán[1], J. Galindo Galindo[1] and E. Fernández Ramírez[2]

[1]The National Institute for Nuclear Research (ININ), Mexico

[2]Universidad Alfa Lambda, Mexico

Radioactive and nuclear wastes containing fission products such as Nb-94 or Fe-55, weak emitters of X-rays and gamma rays, with half-lives of 20300 and 2737 years, respectively, are difficult to quantify directly and therefore must be separated and isolated for its quantification (isotopic characterization). Extraction chromatography (EC) combines the selectivity of liquid–liquid extraction with the multistage character of chromatography. EC is a separation technique frequently used to remove and recover metals from aqueous solutions. It is simple, rapid, highly efficient, low organic solvent consumption, and generates less waste than other separation techniques. The present work proposes the preparation of extraction chromatography materials (ECM) using as stationary phase Amberlite®XAD4 (polymer based on styrene-divinylbenzene, adsorbent of hydrophobic compounds) and PTFE (fluoropolymer of tetrafluoroethylene with excellent hydrophobicity), and as extractant agent MIBK (methyl isobutyl ketone) at different concentrations. Nb and Fe partition data were determined in HCl solutions with the prepared ECM's, using elution analysis and the radiotracers Nb-94 and Fe-59. ECM's were characterized by X-Ray Diffraction, Electron Microscopy, and Infrared Spectroscopy in order to determine their properties and to explain their extraction behavior. AMBERLITE®XAD4 is a spherical amorphous material. MIBK is deposited on the surface of AMBERLITE®XAD4 in form of semi-hexagonal, cubic and irregular crystals, and its concentration increases with the augmentation of MIBK concentration used in the impregnation treatment. PTFE has a crystalline structure and MIBK is embedded in its pores. MIBK is not deposited on Amberlite®XAD4 or PTFE when the MIBK concentration is less than 0.5 M. Niobium and Iron are retained in ECM's: MIBK/AMBERLITE®XAD4 and MIBK/PTFE prepared with 0.1M MIBK, being their distribution coefficients independent of HCl concentration. ECM's prepared with MIBK at 0.001, 1, 3 and 7.9 M, in AMBERLITE®XAD4 and PTFE, do not retain either niobium or iron.

Biography

Fabiola Monroy-Guzmán: Chemical Engineer and Master in Nuclear Sciences from Faculty of Chemistry at the National Autonomous University of Mexico. PhD. from University of Paris XI, France; 20 years of experience in radiochemical separation processes. Founder and leader of the ININ's Radioactive Waste Laboratory. Leaderof projects funded by CONACYT (National Council for Science and Technology, Mexico), IAEA (International Atomic Energy Agency) and UNESCO (United Nations Educational, Scientific and Cultural Organization), focused on the production of radioisotopes for medical purposes,archaeometry and management of radioactive waste. ININ full-time researcher.

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Accepted Abstracts

Operando X-ray spectroscopic study on 3D transition metal oxidesas electrochemical catalysts

Zhiwei Hu[1], Jing Zhou[2], Linjuan Zhang[2], Jian-Qiang Wang[2] and **L. H. Tjeng[1]**

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The flexibility of the electronic and crystal structure and chemical versatility of 3d transition metal (TM) oxides have emerged as promising nonprecious metal-based catalysts for many modern energy storage and conversion technologies because of their robustness, low cost, environmental friendliness and accessibility under the environmental atmosphere.Theoretical description of electrochemical processes is too sophisticated even very simple spinel and perovskite. We discuss some simple physics concepts for the design of electrocatalysts for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and batteries on interplay of the charge-, spin-, orbital-degrees of freedom of 3D transition elements and show our previous successful operando spectroscopic studies on the 3D transition metal oxides.

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Influence of the variation of nitrogen flow on the structure, mechanical and tribological properties of TiAlVN coatings deposited by unbalanced magnetron sputtering

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Universidad de Antioquia, Colombia

Ti_6Al_4V alloy is used for the manufacture of orthopedic implants and different parts in the automotive and aeronautical industry. However, its limited hardness and wear resistance has led to its surface modification through plasma nitriding and / or the application of hard coatings such as TiN, TiAlN and TiAlVN, among others, improving their tribological behavior. Most of the published works report TiAlVN coatings deposited from independent targets of $Ti_{50}Al_{50}$ alloy and pure vanadium or from $Ti_xAl_yV_z$ alloy targets with high aluminum and vanadium contents. In this work, the development of a TiAlVN coating using a target of the Ti_6Al_4V alloy deposited on substrates of the same alloy was proposed using the unbalanced magnetron sputtering technique in order to eliminate the costly process of plasma nitriding, which normally takes place at temperatures between 600 and 800°C. The deposition of the coatings was performed by modifying the nitrogen flow with 0, 6, 7, 8 and 9 sccm and leaving the other process parameters constant. The effect of the modification of the N_2 flow on the microstructural, mechanical and tribological properties was evaluated, finding that small changes in the N_2 flow have a marked influence on the microstructure of the coating, passing from a biphasic coating α-Ti and β-Ti of the Ti_6Al_4V to a biphasic TiN + Ti_2N for low nitrogen flows and finally to a single phase TiN coating for the highest nitrogen flow of 9 sccm. The increased flow of N_2 in the mixture with argon led to a TiAlVN coating of less roughness and grain size, as well as greater hardness and wear resistance compared to Ti_6Al_4V, and even higher than the values reported in the literature for the TiN. These results demonstrate that this technological strategy can replace the plasma nitriding of Ti_6Al_4V.

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Failure mechanisms of APS-YSZ-CoNiCrAlY thermal barrier coating under isothermal oxidation and solid particle erosion

R. Liu[1], S.K. Essa[1], K.Y. Chen[2] and **X.J. Wu[2]**
[1]Carleton University, Canada
[2]National Research Council of Canada, Canada

The high temperature oxidation and solid particle erosion of air plasma sprayed-thermal barrier coating (APS-TBC) system was studied experimentally. The APS-TBC consists of an 8 wt% yttria partially stabilized zirconia (YSZ) top coat and CoNiCrAlY bond coat deposited on Inconel 718 substrate via atmospheric plasma spraying process. Isothermal oxidation tests of APS-TBCs were conducted at 1050°C, 1100°C and 1150°C in air for up to 1970 hours. Solid particle erosion tests were also conducted for both as-deposited and isothermally exposed TBC specimens at selected particle impingement angles and velocities at ambient temperature. The scanning electron microscopy (SEM) shows the formation of thermally grown oxide (TGO) scale due to oxidation of CoNiCrAlY bond coat, and the oxidation kinetics of TGO growth is described by the parabolic rate formulae. The failure of APS-TBC system under isothermal oxidation is associated with the spallation of the top coat through propagation and coalescence of cracks along the coating interface affected by the TGO growth. The solid particle erosion rate of the top coat was found to increases with the impingement angle, and reaches the maximum erosion rate at normal impingement of particles. The erosion resistance of the APS-TBC was observed to increases after TBC specimen were exposed at 1100°C and 1150°C for 72 hours, probably due to the sintering effect on the top coat resulting in reduction of top coat porosity.

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Paramylon: Processing routes for materials applications

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[2]Université de Reims Champagne-Ardenne, France

[3]UFR Sciences Exactes et Naturelles, France

Unlike many polysaccharides produced by microalgae, for which cheaper alternatives exist from macroalgae or plants, paramylon from Euglena gracilis presents a unique macromolecular structure. This reserve glucan produced in the form of intracellular granules by the green microalgae contains only linear □(1-3) linkages, resulting in the formation of triple helix by the polymer chains and a very high crystallinity.

Processing and purification for applications as biomaterials requires the use of efficient and non-derivatizing solvents. While strong acids tend to induce depolymerization, strong bases have been showed to allow preserving the triple helix structure for the production of nanofibers. Recently, a commercial imidazolium ionic liquid was successfully used for solubilizing paramylon granules into biomaterial films for wound healing. As designed solvents, Ionic Liquids (ILs) may be used not only for such final polysaccharide shaping step, but also upstream during the extraction. For this purpose, we evaluated the solubility of paramylon in different biobased ILs. These ones have been synthesized combining choline hydroxide or choline esters with carboxylates derived from biobased acids or amino acids. The solubilization tests of the paramylon have been performed at different temperatures using sometimes ultrasounds. The influence of a co-solvent (water or ethanol) was also studied and the best conditions are mild and in total accordance with green chemistry principles. The regenerated powder of the biopolymer was then analyzed via 13C NMR spectroscopy and X-Ray Diffraction; no chemical modification was observed overall, Furthermore, the IL can be recycled. From our results, we can state that the biobased ILs were at least as efficient as commercial immidazolium ionic liquids. Our biobased ILs are thus good candidates to extract and process paramylon as biomaterials.

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Influence of modifying palladium nanoflower-type coating on low-temperature hydrogen permeability through Pd-Ag membranes

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Palladium based membranes are used to produce high-purity hydrogen. One of the ways to modify the membrane surface is to create a nanostructured layer using powdered hydrogen chemisorbing substances. The aim of this study has been manufacturing of resistant to long-term use palladium-containing films, modified with a pentagonally structured nanoflower-typecoating, capable of transferring hydrogen at low temperatures. This will reduce energy costs in the process of obtaining high-purity hydrogen, as well as use the developed membranes to create a hydrogen electrode of an oxygen-hydrogen fuel cell operating at low (0-100°C) temperatures.

During the study two methods of surface modification have been obtained: the classical method of palladium black "nanoparticles" and the new author's method "nanoflower". Pentagonally structured palladium nanocrystalliteshave been obtained by the electrochemical method from a working solution containing a surfactant (tetrabutylammonium bromide). A necessary condition for obtaining such structures has been a reduced current density compared to the classical palladium black method.

Thin palladium-silver films with a thickness of 10 μmhave been modified on both sides by the developed coatings. After that, the films as membranes have been studied in the processes of hydrogen permeability. The values of the hydrogen flux for membranes modified by the "nanoflower" method are approximately 1.8 times higher than those for membranes obtained by the classical palladium black method. An important feature of the experiment has been the increased flux despite the reduced real surface area. The feature has been recorded in membranes with a lower roughness, but with a pentagonally structured surface organization. This have occurred contrary to the classical concepts of acceleration of the surface stages of hydrogen transport, which indicate that there is no alternative to an extensive increase in the development and specific surface area of palladium membranes.

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EBSD Study of delta-processed Ni-based superalloy

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Nickel-based superalloys are extensively used in the aerospace and power generation industries due to their excellent mechanical properties at elevated temperatures and good corrosion resistance. Typically, these alloys require accomplishing critical standards during their manufacturing process. In this study, an Inconel 718 (IN718) Ni-based superalloy was subjected to a delta-processing treatment (DP718) and subsequently deformed at high temperature. Samples were compressed below and above the δ-solvus temperature at two different strain rates of 0.001 s^{-1} and 0.01 s^{-1}. A detailed microstructural characterization was carried out by the electron backscattered diffraction technique (EBSD). Kikuchi patterns and the orientation relationship of the δ-phase were identified. For samples deformed above the δ-solvus at 0.01 s^{-1}, an increase in the percentage of low angle grain boundaries (LAGB) within deformed grains and a decrease in high angle grain boundaries (HAGB) were observed. Comprehensive observation of the microstructural evolution of IN718 subjected to DP718 using orientation map images was also performed.

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Optical and electrical properties of CdS: Cu thin films synthesized by CBD and SILAR technique

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The interesting properties of semiconductor materials have a wide field of application as thin-film components in various devices such as radiation filters, photosensors and some types of photovoltaic structures. CdS is a very interesting semiconductor material for its application in optoelectronic devices. As part of a polycrystalline solar cell, CdS acts as a window layer for solar radiation. On the other hand, efficient electronic components based in this material such as photodiodes or LDR photoresistors are produced and marketed. The optical and electrical properties of thin films of CdS synthesized by the chemical bath deposition technique (CBD) can be tuned by controlling growth parameters and / or post-synthesis processing for doping with metals such as Cu, Ag and Al among others. In this work, CdS thin films doped with Cu were obtained through two stages. In the first one, a free ammonia CBD reactor was used. For the synthesis of the CdS simple film, reagents such $CdCl_2$, $Na_3C_6H_5O$, KOH and CH_4N_2S were used at 70°C, with a deposit time variation of 30, 60, 90 and 120 minutes. Subsequently in the second reactor, the films were doped by the SILAR technique at 24°C by immersion in an aqueous solution of $CuSO_4$.

For the optical characterization of the thin films, a UV-Vis HACH DR6000 spectrophotometer and Photoacoustic Spectroscopy were used, using a 900W Spectra-Physics model 66885 xenon lamp, an Oriel Cornerstone 130 monochromator and an MTEC 300 photoacoustic cell. With these techniques, absorption and transmission spectra in the range of 250 to 1200 nm were obtained, as well as the energy of the bandwidth of bandgap (Eg). The electrical properties such as the concentration of charge carriers and mobility, resistivity and electric conductivity, were determined using the HMS-3000 Hall effect measurement system. Likewise, the I-V curves were obtained and the TLM method was applied to measure the laminar resistance of the materials.

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Potential use of Jamaica flower (Hibiscus sabdariffa) waste as a reinforcement of cornstarch films

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Natural polymers have emerged as an important source to develop alternative plastics. Due to the availability and biodegradation, these materials promise to be an important contribution for sustainability. However, the main disadvantage of these materials are their poor mechanical and thermal properties. One way to improve the properties of natural polymers is using fibers as a reinforcement, but synthetic fibres can cause health problems and are also difficult to recycle. One solution is the synthesis of composites using bio-renewables resources. Jamaica flower (Hibiscus sabdariffa) is an annual fibrous plant very cultivated and used around the world, but after the culinary use Jamaica flower became a waste. Recent studies are focused on the potential use of these wastes. Thus, this research is concerned on reuse of Jamaica flower waste for the development of polymer composites with cornstarch. The variables are: reinforcement content and plasticizer content. Reinforcement were added separately at 2, 4, 6, 8 and 10 wt% to the starch matrix and the composites were processed by a casting/solvent evaporation method. The morphological characteristics, mechanical and thermal properties of the matrix and composites were studied by scanning electron microscopy, thermogravimetric analysis, differential scanning calorimetry and dynamic mechanical analysis. The morphology, evaluated by scanning electron microscopy, indicated a uniform dispersion of jamaica in the starch matrix as a result of good compatibility between these biopolymers, also corroborated by FTIR. The morphological characteristics, thermal and thermo-mechanical properties of the materials reveal the development of new green composites with better properties than the original matrix.

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Dynamic nanostructuring in premelting phase of ionic crystals

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Appearance of the transient states near the melting point as a rule has been accompanied by anomalous behavior of different parameters at temperature increasing (heat capacity, thermal conductivity, electroconductivity, selfdiffusion coefficient, surface melting etc.). Transient processes during melting (premelting effect) are considered as a fundamental process and are observed in materials with different types of chemical bonds. In this work, were analyzed the structuring dynamics of the transient premelting phases of ionic crystals (KCl, NaCl). It was revealed that the premelting is a nonequilibrium fluctuation process accompanied by the appearance of dissipative states near the melting point in the temperature area $T \geq 0.8$ Tm. Studies of the spectral characteristics of fluctuation thermal processes have shown that the frequency spectrum of such fluctuations is $1/f^2$ noise or nonlinear Brownian noise. Unlike white noise, Brownian noise is correlated, which indirectly indicates structural transformation in the premelting phase.

Structural studies by X-ray diffraction (XRD) in the premelting region of KCl and NaCl also revealed a nonmonotonic change in the intensity of peaks and sizes of coherent-scattering regions at different temperatures. Based on the data of X-ray structure analysis, the sizes of coherent-scattering regions (~60-90 nm) in the premelting region of KCl, NaCl were estimated. The KCl XRD patterns, a broadening of the KCl (200) reflection is observed in the premelting temperature range. This indicates the decomposition of large crystals of KCl into nanoclusters near the melting point. The results of estimating the crystallite size in the KCl premelting phase show that the coherent-scattering regions size in the transition phase changes nonlinearly in the premelting temperature range.

Thus, increase of heat fluctuations near T_m reduced to dynamic formation of nanocluster structures (generation of dissipative structures or ordering through fluctuations).

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Terbium(III) chelates-carbon dots nanohybrids as a highly sensitive intracellular temperature and pH sensors

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A new nanomaterial based on PSS-[$Tb_2(TCAn)_2$] was synthesized by solvent-induced nanoprecipitation for highly sensitive intracellular temperature monitoring within the physiological 303-313 K range. The degree of bromination of TCA ligands was found to play a dramatic role in control of thermoresponsive behavior of PSS-[$Tb_2(TCAn)_2$] particles. Tetra-brominated thiacalix arene based nanoparticles provided the most sensitive response to the heating, but restricts their applicability to the single use. However, the di-brominated ligands provide the optimal ligand environment of the Tb^{3+} ions in the nanoparticles for the recurrent temperature measurements for the five "heating-cooling" cycles at least.

Effective cell internalization, low cytotoxicity, and bright green Tb^{3+}-luminescence provides great potential for *in vivo* intracellular monitoring of temperature changes induced by hyperthermia or pathological processes in narrow range of physiological temperatures with unprecedented sensitivity (SI=5.25%K^{-1}), and may represent a significant step forward for accurate 2D temperature mapping.

Aiming at ratiometric temperature sensing, second luminescent component, namely carbon dots (CDs), was introduced to the nanoparticles. Resulting hybrid PSS-[TbL-CD] nanoparticles showed excellent colloidal stability, bright and reversible thermo responsive and pH responsive functions in green (545 nm, $^5D_4$-$^7F_5$ transition of Tb^{3+}) and blue (450 nm, designated to CD fluorescence) regions of spectrum, correspondingly. Temperature sensing was achieved via green peak reversible quenching, while blue peak remained unchanged. Oppositely, CD fluorescence peak demonstrates sensitivity to pH changes in the range of 5-7.5 where 545 nm peak shows constant intensity. Dual function nanosensor constructed via combination of Tb^{3+} chelate and CDs within one nanoarchitecture allows remote real-time monitoring of two main parameters, temperature and pH, in cells at nanoscale dimensions.

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Carbon nanotube concentration effects on the elelctro-optic properties of liquid crystals

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The major objective of this study wastoimprove the quality of liquid crystal devices by using carbon nanotubes. The concentration of inserted particles is crucial for the electro-optic properties and doesn't present a continuous behavior suggesting a bundling process after a critical value (about 0.5% mass fraction of MWCNT). This paper is aimed to qualitatively explain the electro-optic behavior of nematicliquid crystals with carbon nantubes dispersions at different temperatures in the nematic range for low concentration (below 0.5%massfraction) and for high concentration(above 0.5 mass fraction).

The analyzed samples were prepared by mixing 7CB nematic with multiwalled carbon nanotubes. The nanotube's length is between 0.1 to 10 micrometers, the inner diameter is 2 nm – 6 nm and the outer one is about 10 nm to 15 nm. The samples were mixed in two concentrations 0.36% and 1.3% (mass fraction) and used to fill 15 micrometers thick planar aligned cell. To determine the electric Freedericksz transition threshold, a laser beam was sent through the sample subjected toan external electric field. The emergent beam intensity was recorded and plotted versus the applied field.

The Freedericksz transition decreases with the CNT adding if the concentration is lowand increases for high concentration when compared to simple 7CB samples. This suggests a bundling phenomenon occurs in high concentration and theinteractions with the host molecules and the applied field is different. The most important aspect observed is a decrease of the Freedericksz transition threshold when small amounts of MWCNT are added. For high nanoparticles concentration, the transition threshold is increased due to the bundling effects.

Superconductivity in graphene monolayer calculated via Kubo formula

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We employed the massless Dirac's fermions formalism together with the Kubo's formula of the linear response theory to study the transport by electrons in the graphene monolayer. We calculated the electric conductivity and verified the behaviour of the AC and DC electric conductivities of the system that is known to be a relativistic electron plasma. Our results show a behaviour of the AC conductivity tending to infinity at DC limit and therefore a superconductor behaviour to the electron transport at low-temperature.

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Poly(gyceric acid ether): A new 3,4-dihydroxyphenyl derivative of polysaccharide from medicinal plants, its synthetic analogues and their comparative anticancer efficacy

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The main chemical constituent of high molecular (>1000 kDa) water-soluble preparations from medicinal plants of *Symphytum asperum, S.caucasicum, S.officinale, S.grandiflorum, Anchusa italica, Cynoglossum officinale* and *Borago officinalis* (Boraginaceae) according to data of liquid-state ^{1}H, ^{13}C NMR, 2D $^{1}H/^{13}C$ HSQC, 2D DOSY and solid-state ^{13}C NMR spectra was found to be poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDPGA). The polyoxyethylene chain is the backbone of this regular polymer with the repeating unit 3-(3,4-dihydroxyphenyl)glyceric acid residue. PDPGA as a 3,4-dihydroxyphenyl derivative of poly(glyceric acid ether) belongs to a novel class of acidic polysaccharides (sugar acids) as well. Its basic monomeric moiety glyceric acid is a natural three-carbon sugar acid which is oxidative form of aldotriose glyceraldehyde. The monomer of PDPGA 3-(3,4-dihydroxyphenyl) glyceric acid was synthesized via Sharpless asymmetric dihydroxylation of trans-caffeic acid using a potassium osmate catalyst which is new findings in sugar acids. Methylated derivative of PDPGA was synthesized via ring opening polymerization of 2-methoxycarbonyl-3-(3,4-dimethoxyphenyl)oxirane using a cationic initiator (BF_3•OEt_2). Human Hyaluronidase (Hyal-1) degrades high molecular mass Hyaluronic acid (HA) into smaller fragments which have pro-inflammatory effects. PDPGA possesses the ability to inhibit the enzymatic activity of Hyal-1 completely. Consequently PDPGA exhibited anti-inflammatory efficacy. PDPGA and its synthetic monomer suppressed the growth and induced death in androgen-dependent (LNCaP) and -independent (22Rv1) human prostate cancer (PCA) cells. PDPGA induced apoptotic death by activating caspases, and also strongly decreased androgen receptor and prostate specific antigen (PSA) expression. In 22Rv1 xenograft model male athymic nude mice with 22Rv1 xenografts was administered orally of PDPGA. Plasma analyses revealed that PDPGA administration caused a strong dose-dependent decrease in PSA levels by 87%. Anticancer efficacy of PDPGA against PCA cells is more compared to its synthetic monomer. Methylated PDPGA did not show any activity against PCA. Overall, this study identifies PDPGA as a potent agent against PCA without any toxicity.

Highly efficient flexible perovskite optoelectronic devices with inorganic nanopillar arrays

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One-dimensional (1D) nano-arrays can reduce light reflection loss, suppress recombination dynamics, guide charge carrier transport, andrelax stress and strain in flexibleoptoelectronic devices, to improve optoelectronic function and stability under aging and mechanical bending. However, *in-situ* fabrication of 1D nano-arrays on polymer-based flexible electrodes is challenging, mainly due to degradation of the flexibleelectrodes at high temperature of in-situgrowth.

Here, nanopillar arrays (NaPAs) made of diverse inorganic materials, such as Ti, TiO_2, SnO_x(functioning aselectron transporting layers) and NiOx (serving as hole transporting layers), are deposited onto a flexible electrode by glancing angle deposition (GLAD), to create perovskite solarcells (PSCs) and photodetectors. As-grown NaPAs enhance light transmittance, facilitate light harvesting in perovskite, promote charge carrier transport and collection, and facilitate the formation of large perovskite grains. All these features lead to high efficiency of >20% and >17% for the rigidand flexible PSCs, respectively. No obvious cracknucleationisformedonthe NaPAsafter500 bending, resulting in good mechanic stabilityof the photovoltaic performance. Furthermore, compared to the conventional mesoporous counterparts, metallic oxideNaPAsenable the perovskite photodetectors to comprehensively enhance the detection speed, responsivity, and detectivity, and to extend the linear dynamic range.

We devise an advanced technique of low-substrate-temperature GLAD generally adapted to *in-situ* deposition of charge carrier transporting layers made of inorganicNaPAs on flexible electrodes, to significantly enhance optoelectronic performanceof flexible devices.

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Nonlinear modelling of hierarchical ZnO nanoforms formation

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The polymorphic transitions of ZnO at the nanoscale was studied from the perspective of stability of polyhedral clusters at the nanoscale. It is shown that in a gaseous environment among cubic, hexagonal prism, spherical, octahedral, icosahedral clusters with primary structures of *B*3, *B*4 and *B*1 in the size range from 7 to 500 atoms only octahedral clusters $Zn_{146}O_{140}$ and $Zn_{85}O_{80}$ pass geometry optimisation while approximately preserving the initial crystal structure. These octahedral clusters showed stability for more than 1 ps as a result of molecular dynamics simulations at temperatures from 70 to 1500 K. The PM6 parametrisation method was used for calculations.

Due to the compatibility of the [111] plane of a *B*3 ZnO crystal and the [0001] plane of a *B*4 ZnO crystal a model of a symmetry-driven transformation at the nanoscale is proposed. An octahedral core provides four tetrahedrally oriented growth plains that define the symmetry of four interconnected ZnO crystals of the *B*4 polymorphic modification, thermodynamically stable at normal conditions.

Defining the transformation area as a formation centre and using nonlinear models of multi-element dynamic system self-assembly the formation of hierarchical ZnO nanoforms such as ZnO tetrapods can be described.

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Vertical graphene network: Synthesis and applications

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Graphene-based nanostructures are recognized as smart materials and have attracted much attention due to their outstanding properties as well as emerging applications. Among them, vertical graphene network (VGN) with large surface area could be promising material as a platform for electrochemical and bio applications. VGN is composed of few-layer graphenes standing almost vertically on the substrate to form self-supported 3-dimensional structure. VGN and similar materials can be synthesized by plasma-enhanced chemical vapor deposition (PECVD) on heated substrates (600-800°C) using methane and hydrogen mixtures. The height of VGN increases almost linearly with the growth period, while the thickness of each sheet and interspaces between adjacent sheets are almost constant. VGN is sometimes decorated with nanoparticles and biomolecules. The maze-like architecture of VGN with large-surface-area graphene planes would be useful as electrodes for energy storage devices and scaffold for cell culturing. Especially, combined with surface functionalization including surface termination and decoration with nanoparticles and biomolecules, VGN can be suitable as platform in electrochemical and bio applications.

Most important factors affecting morphology, crystallinity and growth rate of VGN are the balance between carbon precursors and H atoms in the plasma,and ion energy/flux incident on the substrate as well as on the growing surface. Morphology of carbon nanostructures should be controlled according to their applications. We report the current status of the synthesis of VGN using several PECVD techniques, and focus on the control of their structures during the growth processes as well as surface decoration to be used as platform of the electrochemical and bio applications. Electrochemical experiments demonstrate that VGN offers great promise for providing a new class of nanostructured electrodes for electrochemical sensing, biosensing and energy conversion applications.

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The influence of deposited molecular layers amount on the morphology and optical properties of MoS_2 nanostructures

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Our research shows the influence of the amount of deposited molecular layers on the morphology and optical properties of MoS_2 nanostructures formed during the gas transport transfer of sulfur vapors to the hot zone of a reactor with metallic molybdenum and subsequent deposition on a mica substrate (muscavite). Our previous experience has shown that the temperature of gas transport synthesis of MoS_2 nanolayers should not exceed 800◦C.

By this time, we obtained MoS_2 nanostructures of various thicknesses, starting from the monomolecular layer, in the temperature range of 525-600◦C. Results of research using atomic force microscopy AFM, optical absorption spectroscopy and Raman spectroscopy of MoS_2 nanostructures of different thickness show that in the range of 525-600◦C it is possible to obtain MoS_2 monomolecular layers containing trigonal domains with D_{3h} symmetry and having a band gap of 1.84 eV at a straight-band optical transition with the formation of excitons at room temperature. The thickness of one molecular layer of MoS_2 is equal to 0.625 nm.

The two-layer films obtained under the same conditions contain domains of hexagonal symmetry D_{6h} of micron sizes. In some areas of such films the top layer of MoS_2 is folded into nanotubes several tens of microns long. With an increase in the number of deposited molecular layers, small trigonal domains self-organize during growth into quantum dots of average diameter of about 50 nm, located at medium distances100-200 nm from each other.

The next step in self-organization is formation of fractal-like structures of MoS_2 with trigonal and hexagonal fragments. In the Raman spectra of these structures, the values of the modes of intra-layer and inter-layer vibrations E^1_{2g} (377.5 cm^{-1}) and A^1_g (403.8 cm^{-1}) differ not only from the corresponding values of the modes of the monomolecular layer, but also from all known values of bulk samples. The frequency of the intra- layer mode in these samples E^1_{2g} has the lowest of all known values and is due to the intermediate dimension of the fractal substructures between 2D and 3D.

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Role of exchange excitons in organic optoelectronic devices

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Most organic and perovskite optoelectronic devices, such as organic solar cells (OSCs), perovskite solar cells (PSCs), organic light emitting diodes (OLEDs) and organic photo detectors (OPDs), involve either charge generation or light emission or both which occur at the interfaces between a donor (D) and an acceptor (A). It is this interface where the charge transfer (CT) excitons are generated in OSCs, PSCs and OPDs from the photo excited excitons and in OLEDs by recombination of injected charge carrier pairs. The charge transfer(CT) exciton states have been well identified as precursors for charge generation in OSCs and charge recombination in the thermally activated delayed fluorescence (TADF) based (third generation) OLEDs.

There are two issues of very significant importance which have not yet been resolved: (i) Zhang et al. have reported 100% internal quantum efficiency from purely organic based TADF OLEDs, which means triplet excitons recombine radiatively without the aid of any heavy metal atoms and that means very weak spin-orbit coupling. It is very puzzling that without the significant strength of spin-orbit coupling how can triplet excitons recombine radiatively. (ii) Although the operation of OSCs and OLEDs is reversible, both the operations have not yet been achieved in a single device.

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SEM-EDS analysis of adscititious layers in partitions historical buildings

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The aim of the study was a qualitative analysis of the composition of adscititious layers in partitions historic buildings, taking into account the differences in the microstructure of the tested composites. Representative material samples were taken for the tests, all of them were taken from the historical structural fragments of brick walls of the Bishop's Castle and the Roman Catholic Church of St. John the Baptist in Janow Podlaski. The samples were dried at room temperature and then placed on a carbon tape. In the surface and point analyzes, an accelerating voltage of 15 kV was used, the samples were not sputtered with conductive material. Based on the results of SEM-EDS analyzes for various areas of the studied samples of supplementary material, it can be concluded that the main elements included in the tested samples are: silicon, carbon, calcium, as well as aluminum, iron, potassium and magnesium. In addition to the exchangeable elements, the material tested also contained small amounts of sodium, sulfur and chlorine. The Hitachi TM3000 scanning microscope was used to determine the chemical composition in the micro-area of the main mineral components of the examined supplementary layers, equipped with a chemical composition analysis system based on X-ray energy dispersion - EDS by Swift ED 3000 Oxford Instruments. The elemental composition of the samples taken is a consequence of the chemical composition of the original clay deposits used to make the brick. The oxide composition of such deposits is: Al_2O_3, SiO_2, Fe_2O_3, MgO, CaO, Na_2O and K_2O. A significant amount of silicon and aluminum was due to the presence of aluminosilicates, the main material of brick clay. The presence of iron confirmed the presence of oxides of this metal in the composition of the supplementary layers, mainly Fe_2O_3, giving the material a characteristic brown-red color. The uniform presence of most elements (except S, Na) in the complementary layer indicated a similar elemental composition of the complementary layer with the parent material. The particle distribution of most elements coincided with each other. Directly in the supplementary layer, more calcium and a smaller amount of silicon were visible, which may indicate that it was a separate technological layer, but with a similar composition to the substrate.

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Influence of the interlayer temperature on structure and properties of wire and arc additive manufactured duplex stainless steel product

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WAAM (wire and arc additive manufacturing) is becoming an increasingly popular method to produce components from metals, which are usually not so suitable for conventional production methods. One of the good examples is duplex stainless steels (DSSs), which are quite complex for welding and machining. Excessive ferrite amount is a common problem for them and controlling an interlayer temperature could offer a solution. However, using too low interlayer temperature will slow down the whole process and compromise one of the WAAM's main advantages—the high productivity. The aim of this study is to find the relationship between interlayer temperature and process duration and to determine the influence of the interlayer temperature on product structure and other properties. Three samples (walls) were made using different interlayer temperatures (50°C, 100°C and 150°C) and they were tested to analyze their surface texture, chemical composition, ferrite amount, the appearance of porosity and the hardness. Ferrite amount was higher and there was more porosity on lower interlayer temperatures, while there is no significant difference between surface texture and chemical composition for the samples. Considering the fact that higher interlayer temperatures provide a faster process, they should be preferred to produce duplex stainless steel products.

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Equine collagen as emerging material for biomedical applications: New trends and latest updates

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Being the most abundant structural protein of vertebrates extracellular matrix, type-I collagen always aroused great interest in the field of life-science and bioengineering, thanks to its intrinsic favorable structural properties and bioactivity. Commonly used sources of collagen are represented by bovine and swine but the zoonosis transmission risks, the immune response and the religious constrain limited their use. Thus, type-I collagen isolated from horse recently gained increasing interest as an attractive alternative, so that, although bovine and porcine derived collagens still remain the most common ones, more and more companies started to bring to market several equine collagen-based products for healthcare applications. For this reason, in the last five decades equine collagen behavior and reactivity started to be in-depth studied in order to manufacture different types of medical products. Advanced investigation techniques (e.g. HPLC-MS, AFM, DSC, CD, TEM, WAXS, SAXS, FT-IR) allowed to highlight the peculiarities of this type of collagen compared to the others on the micro-, nano- and atomic scale and to control its hierarchical organization at all processing steps (from collagen extraction to the device final sterilization) in order to develop collagen-based devices with finely controlled application-related end-properties besides enhanced bioactivity. Thus, our aim is to stress the advantages and disadvantages deriving from the use of equine collagen for the manufacture of Tissue Engineering Medical Products (TEMPs)followed by a brief insight on the requirements that a medical device must meet before being commercialized, supported by our evidences and ten-years know-how. Lastly, clinical trials and current uses in the biomedical field will be argued.

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Exfoliation corrosion of Mg-14Li-1Ca alloysexposed to marine atmosphere for one year

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Magnesium (Mg) and its alloys hold promising applications in automotive, 3Cproducts (computer, communication and consumer Electronic) and biomedical fields due to their low density, high damping capacity, good castability and recyclability as well as excellent biocompatibility. However, they are prone to corrosion in aggressive solutions. The low corrosion resistance of Mg alloys is a major concern for extensive utilization, especially for load-bearing structure materials. So far, exfoliation corrosion of magnesium alloys has scarcely been reported. The microstructure, compositions and constitutes of as-extruded Mg-14Li-1Ca alloy has been investigated using field-emission scanning electron microscopy (SEM), EDS, X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectrometry (FTIR) together with X-ray diffractometer (XRD). Electrochemical impedance spectroscopy and polarization as well as hydrogen evolution tests are applied to reveal the corrosion mechanisms. Results show that's evere exfoliation corrosion occurs on extruded Mg-14Li-1Ca alloys exposed to marine atmosphere in a sea island field for almost one year. The findings are due to the elongated microstructure, and delamination or peeling off of the lamellar structure caused by galvanic and wedge effects. Galvanic effect between Mg_2Ca particles and their neighboring α-Mg matrix facilitates preferred dissolution of Mg_2Ca particles prior to α-Mg matrix; wedge effect is caused by the formation of corrosion products and hydrogen evolution.

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Spin based electronics, a new era in science and technology: Role of DMS and nanocomposite materials

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We have entered in a new age of technology, where the transport of elementary particles will be driven by its spin degree of freedom. A new electronics, which is completely based on 'spin' of electron popularly known as 'Spintronics' is a subject of current research. The basic materials required for such technology is a daunting task to materials scientists.

In this talk after introducing briefly the motivation of this new technology, I will highlight the research works carried out in last decade related to (i) diluted magnetic semiconductors (DMSs) a basic material for future spintronics and (ii) metal-insulator nanocompoaites a promising materials for manipulating electron's spin motion. Ion implantation has been identified as an important tool to synthesize diluted magnetic semiconductor (DMS) materials. Synthesis of transition metal implanted ZnO as a DMS material, and their ferromagnetic properties from intrinsic to extrinsic regime will be discussed. Origin of ferromagnetism (due to substitution of transition metals in ZnO) probed by a combined study of X-ray absorption (XAS), X-ray magnetic circular dichroism (XMCD), X-ray photo electron spectroscopy (XPS), X-ray diffraction (XRD) and SQUID will be highlighted. Finally, shape engineering of magnetic nanoparticles embedded in insulating matrix and trigeering exchange bias, anisotropy and quantum mechanical tunneling of electrons will be discussed. Results will explained in the framework of thermal spike model and density functional theory.

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Carbon nanotubes produced by HiPCO process in nanopharmaceuticals applications

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During the past years, carbon nanotubes (CNTs) have attracted considerable interest since their first discovery great progress has been made in the field of nanomaterials given their great potential in biomedical applications. Carbon nanotubes (CNTs), due to their unique physicochemical properties, have become a popular tool in cancer diagnosis and therapy. They are considered one of the most promising nanomaterials with the capability of both detecting the cancerous cells and delivering drugs or small therapeutic molecules to these cells Because of the unique structure, extremely high specific surface area to-volume ratio enables them to use in an intense real time applications such as detection and treatment of cancerous cells, nervous disorders, tissue repair. and excellent electrical and mechanical properties carbon nanotubes composed of excellent mechanical strength, electrical and thermal conductivities makes them a suitable substance toward developing medical devices. CNTs have been explored in almost every single cancer treatment modality, including drug delivery with small nanomolecules, lymphatic targeted chemotherapy, thermal therapy, photodynamic therapy, and gene therapy and demonstrate a great promise in their use in targeted drug delivery systems, diagnostic techniques and in bio-analytical applications. Majority of the biomedical applications of CNTs must be used after successful functionalization for more potential applications than pristine CNTs. There are several approaches to modify pristine CNTs to potentially active. CNTs poised into the human life and exploited in medical context. Here in, we reviewed the following topics (i) Functionalization of CNTs (ii) CNTs in real time applications such as drug delivery, gene therapy, biosensors and bio imaging; (iii) CNTs 3D printed scaffolds for medicine and (iv) Biocompatability and Biodegradability. Single-walled carbon nanotubes (SWCNTs) were synthesized using the high-pressure carbon monoxide disproportionation process (HiPCO). The SWCNT diameter, diameter distribution and yield can be varied depending on the process parameters. The obtained HiPCO product present an iron nanoparticle encapsulated heteronanocarbon (core-shell

nanoparticles) at low pressure (1bar) after removing of iron metal catalyst nanoparticle and amorphous carbon by acid immersion and oxidation. The resulting therapeutic molecule in the form of core-shell nanoparticles and single walled carbon nanotubes after functionalization by filling of iron can be use as therapeutic nanomaterials in nanomedicine in diagnosis and treatment of cancer tumor. This paper describes the synthesis method and role of multifunctional nanoparticle in diagnosis and treatment of cancer. Therefore, the aim of this review is to provide basic information on nanoparticles, describe previously developed methods to functionalize nanoparticles and discuss their potential applications in nanobiomedical and mention the therapeutic nanoparticle large scale production and commercialization challenges. In the final part of the review, emphasis is given on the pharmacokinetic aspects of carbon nanotubes including administration routes, absorption mechanisms, distribution and elimination of carbon nanotubes based systems. Lastly, a comprehensive account about the potential biomedical applications has been given followed by insights into the future carbon nanotubes from synthesis to in vivo biomedical applications.

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Baromagnetic effect in antiperovskite Mn_3GaN compound Cong Wang

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The antiperovskite(Mn, Fe)3XN(C,B) (X: Zn, Ga, Sn, Cu, etc.) compounds display rich physical properties, such as superconductivity, giant magneto resistance, near zero temperature coefficient of resistivity (NZTCR), abnormal thermal expansion, magneto striction, piezomagnetism, magnetocaloric, ferromagnetic shape memory effect (FSM), abnormal Hall effect (AHE), barocaloric and baromagnetic effects, etc. due to strong "lattice-spin-charge" coupling. It will become a new family for advanced multifunctional materials after the intensive and comprehensive studies on perovskite ABO_3 compounds. There exist abundant magnetic structures, including non-collinear, frustration and spin glass magnetic configurations in this kind of compound. Baromagnetic effect was reported in antiperovskite structured Mn3GaN compounds. The baromagnetic effect at different pressures and temperatures are studied in $Mn_3Ga_{0.95}N_{0.94}$, which is represented by the parameter (Δmp), i.e. the difference between the data at different pressures with the solidifying temperature: Δmp=m(T,p) - m(T,p+Δp). The maximum of the baromagnetic effect under 600 MPa is 2.28 μB. This is the first time to report about baromagnetic effect in antiperovskite compounds.

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Comparative analyses of the thermal properties of biomass briquette fuels of rice husk and groudnut husk

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This work comprised the production, characterization and comparative analyses of biomass briquette fuels produced by blending major agricultural wastes such as rice husk and groundnut husk with coal dust. Different compositions of coal dust blended with rice husk and coal dust blended with groundnut husk briquettes were produced using starch as the binder while $Ca(OH_2)$ served as the de-sulphurizing agent. The briquettes were produced mechanically using a manual briquetting machine with force and compression pressure of 276.36 N and 31.67 N/m2 respectively. The ash content, volatile matter, fixed carbon, moisture content, compressive strength, ignition time, calorific value, water boiling test and burning time were carried out to determine the physical, mechanical and thermal properties of the briquettes. For coal dust/groundnut husk briquettes, the results showed that moisture content values were in the range 2.91 - 5.72%, compressive strength (7.97 - 10.78 N/mm^3), ash content (24.21 - 27.60%), calorific value (22506.81 - 25898.18 kJ/kg), fixed carbon (26.63-48.81 %), ignition time (21.19-38.32 s), water boiling test (2.15-4.94 min) and burning time (16.26-24.34 min). For the coal dust/rice husk briquettes, the moisture content results ranged from 3.37 - 6.95%, compressive strength (9.78 - 12.36 N/mm^3), ash content (16.82 - 21.79%), calorific value (21739.54 - 25921.82 kJ/kg), fixed carbon (27.00-53.71%), ignition time (23.33-41.00 s), water boiling test (1.62-4.12 min) and burning time (16.17-24.15 min). From the result of the work, it could be seen that the briquette blends exhibited improved thermal properties against ordinary coal briquette fuel. Hence, the agricultural waste can be used as an alternative fuel source.

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The influence of filler content and annealing temperature on behavior of melt stretching calcium carbonate polypropylene-based microporous membrane obtained by twin-screw extruder

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Micro-sized calcium carbonate was selected to develop polypropylene-based microporous membranes through MEAUS process (melt extrusion – annealing – uniaxial strain). Different filler percentages were added to polypropylene (1, 5, 10 wt. % calcium carbonate) Parameters such as draw ratio during extrusion, annealing temperature, strain rate, and strain extension were kept as constant in order to analyze the effect of the calcium carbonate, and content of the obtained membranes. The stress applied involved a pre-orientation of the amorphous tie chains prior to crystal chain unfolding, which can be related to the first yield point. A logical pattern of increasing elastic modulus as filler content does is found in calcium carbonate compounds.

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Insight into the structure of non-noble-metal-based electrocatalytic materials by X-ray absorption spectra

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Macroscopic physical and chemical properties of material strongly rely on the coordination structure and electronic structure, involving the evolution of chemical reactants and structural transformation of catalyst during the in-situ chemical reaction process. Exploring the structure in the atomic and molecular level should be supported by in-situ characterization technology, in which synchrotron radiation-based techniques have become an indispensable method. X-ray absorption spectra (XAS) contain rich information concerning the local structure, such as coordination numbers and near-neighbor distances obtained by hard XAS analysis, as well as electronic structure information obtained by soft XAS analysis. In this talk, I will report some works on the application of X-ray absorption spectra in non-noble metal based electro catalytic materials. Our research revealed that the surface structural evolution is crucial for achieving high OER activity.

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Entropy optimization in second grade nanofluids: Importance and significance

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Second Grade Nanofluids have wide applications to both engineering and industry in general, making them important to study. Particularly, we investigate effects of heat transfer and a magnetic field over materials either composed of nanoparticles or coated in nanofluids. Understanding the effects of nanofluid behaviour between rotating disks or over expanding and contracting sheets has profound industrial consequences. An investigation into entropy optimization is conducted and key results pertaining to axial velocity, temperature profiles and magnetic influence are discussed. The work discusses results obtain from modelling using the Cattaneo-Christov heat flux model. The presentation will provide insight into practical applications and inferences of the results arising from research, as well as discussing the mathematical approaches. At the present time, we are also working to develop new results for nanofluid coated materials as part of the manufacturing of more effective Covid-19 face masks.

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Perovskite: A multi-element confinement material

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Perovskite is a major mineral of Synroc material. It is able to confine both alkaline and alkaline-earth elements contained in radioactive waste. Perovskite exists in several crystallographic forms, making them suitable for the confinement of both actinides and alkaline/alkaline-earth elements. The main challenge in the field of sequestration of radionuclides in such crystalline structure is to accommodate great amounts of actinides/lanthanides and alkaline elements, in the same time in perovskite lattice. For this both dry and wet processes of synthesis are experimented. This study summarize many investigations on both simple $Ca_{(1-x-y)}Ce_xSr_yAl_zTi_{(1-z)}O_3$ perovskite (y = 0.04 to 0.16) co-doped with Ce and complexe perovskite $[Ca_{0.91-x}Ce_{0.09}Rb_{0.04}Cs_x[(Zr_{0.50}Ti_{0.45})Al_{0.05}]O_3$, x=0.2 to 0.4], synthesized by dry and route processes. Thorough full structural and chemical durability' characterizations are described for both materials.

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Mathematical modeling and analysis of tribological properties of AA6063 aluminum alloy reinforced with fly ash by using response surface methodology

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Lightweight, high-strength metal matrix composites have attracted considerable interest because of their attractive physical, mechanical and tribological properties. Moreover, they may offer distinct advantages due to good strength and wear resistance. In this research, AA6063 was reinforced with FA particles using compocasting methods. The effects of fly ash content, load, sliding speed and performance tribology of AA6063 –FA composite were evaluated. Dry sliding wear tests were carried out according to experimental design using the pin-on-disc method with three different loads (24.5, 49 and 73.5 N) and three speeds (150, 200 and 250 rpm) at room temperature. Response surface methodology (RSM) was used to analyze the influence of the process parameters on the tribological behavior of the composites. The surface plot showed that the wear rate increased with increasing load, time and sliding velocity. In contrast, the friction coefficient decreased with increasing these parameters. Optimal models for wear rate and friction coefficient showed appropriate results that can be estimated, hence reducing wear testing time and cost.

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Study of optical properties of PVC/ Ag_2O nano-composites by dispersing spherical nanofillers into polymer matrix under normal and heat treated conditions

Aman Kumar and **N.A.Karimi**
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In the present work a novel polymer/metal oxide composites containing Polyvinyl Chloride (PVC) and Ag_2O nanoparticles (NP) were fabricated under room and elevated temperatures. The Ag_2O NP was synthesized by drop wise mixing process having 25 nm in size with spherical surface morphology. The F.T.I.R was taken for (1) virgin PVC film (2) PVC/Ag_2O NC and PVC/Ag_2O (heat treated) Composites. The formation of absorbance peaks, their shifting, intensity and maximum absorbance values were considered in all the three C-C, C-Cl and C-H classified stretching modes of vibrations for different composites. It was found in C-C stretch range the virgin PVC back bone chain occurs at 1101 cm^{-1} which shifted to 1076 cm-1 for PVC/Ag_2O NC, further shift is evident for PVC/Ag_2O (heat treated) Composites at 1151 cm^{-1}. In addition rocking vibration and wagging of methylene group changes in the same fashion. The change in spectral feature takes places due to filling of Ag_2O NP in PVC matrix, indicates that changes in dipole moments occur as a result of molecular vibrations. It is also observed the absorbance peal value is high for virgin PVC film for all modes of stretching vibration, which decreases for Ag_2O/PVC (NC) further decrease is evident for Ag_2O/PVC (NC) heat treated composite..

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Study of the concentration quenching of tris(bipyridine) ruthenium(II) in the silicon dioxide particles

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A study was conducted of the change in the fluorescent properties of the luminescent dye tris (bipyridine) ruthenium (II) chloride (RuBpy) after its incorporation into microparticles of silicon dioxide. A decrease in concentration quenching in saturated solutions of RuBpy after incorporation into silicon dioxide, which occurred during the growth of microparticles in dye solutions, was studied.

Objectives - find out whether the concentration quenching of the tris (bipyridine) ruthenium (II) chloride dye changes after its introduction into silica particles, and if it does, how.

The methods used in the work process - synthesis of silicon dioxide particles according the Stöber method, measurements of absorption, fluorescence and excitation spectra of samples before and after growing the silicon dioxide, interpretation of the results obtained by the MO and coordination chemistry methods, acquiring images of the obtained particles using a scanning electron microscope.

A series of samples were prepared representing the initial solutions of tetraethoxysilane (TEOS), RuBpy, and ammonia in an isopropyl alcohol: water mixture. In this case, the concentration of TEOS and ammonia was constant, while the concentration of the RuBpy increased from sample to sample. The concentration of the most saturated solution exceeded the concentration of the most dilute solution by almost 50 times. A noticeable concentration quenching of the initial solutions is noted, starting with a dye concentration equal to 4.14 × 10-5 mol / l.

Following the work results, the following was established:

1. The sizes of the resulting particles increase in proportion to the increase in the concentration of the dye solution, all other things being equal;
2. The rate of conversion of the starting TEOS ester into silica particles increases in proportion to the increase in the concentration of the dye in the solution, all other things being equal;
3. The introduction of the dye into the nanoparticles of silicon dioxide makes it possible to reduce the concentration quenching by blocking one of the reasons for its formation - the formation of dye aggregates.
4. The fluorescence intensity of the dye solutions increases approximately 3 times after the growth of the silicon dioxide particles, which is associated with an increase in the total turbidity of the solutions and their transition into suspension.

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Directed polymers and interfaces in disordered media and models on random networks

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The investigation of statistical mechanics of disordered systems, random surfaces and membranes has developed a wide set of rigorous and heuristic techniques that have shown a vast space of applicability and rich phenomenology. One of the simplest example of a tethered surfaces are the polymers. In this work we consider field theory formulation for directed polymers and interfaces in presence of quenched disorder. We use the Distributional Zeta Function Method (DZFM) to obtain the average free energy. Under this formalism this quantity is represented as a series of integer moments of the partition function of the model. The structure of field space is analyzed for polymers and interfaces at finite temperature using the saddle-point equations derived from each integer moments of the partition function. For the case of an interface we obtain the wandering exponent also obtained by conventional replica method. Additionally, we study polymers models on random networks, where a pair of polymers on adjacent sites carries a weight factor ω for each link. We relate the network topology and the partition function present in DZFM by using the spectral, disorder and Hamiltonian structure of the system in order to explore the phase diagram, critical behavior, finite-temperature, and finite-size corrections. These kind of models are relevant in polymer science and bioinspired materials.

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Sesquioxide transparent laser ceramics: The current status

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Sesquioxide crystals, such as Y_2O_3, Lu_2O_3 and Sc_2O_3, have cubic crystal structure, relatively high thermal conductivity, small thermal expansion coefficient and small phonon energy. They are considered as a desired host material for high power solid-state laser applications. However, the growth of sesquioxide single crystals is very difficult due to their extremely high melting points (>2400°C). In this talk, we will present our fabrication process for transparent sesquioxide (Y_2O_3 and Lu_2O_3) ceramics with optical quality comparable to single crystals. Rare-earth ions doped Y2O3or Lu2O3raw powders were synthesized by using a chemical co-precipitation method. The powders synthesized in house have high purity (>99.995%) and narrow particle size distribution. The ceramics were first densified in vacuum and then post-treated with a hot isostatic presser (HIP) at below 1600°C, which is only two-thirds of their melting temperature. A series of rare-earth doped sesquioxide-based laser ceramics, such as $Yb^{3+}:Y_2O_3$, $Yb^{3+}:Lu_2O_3$, $Nd^{3+}:Y_2O_3$, $Ho^{3+}:Y_2O_3$, $Er^{3+}:Y_2O_3$, $Dy^{3+}:Y_2O_3$,$Pr_{3+}:Y_2O_3$ and $Cr^{4+}/^{2+}:Y_2O_3$ were fabricated. The fabricated laser ceramics have very good optical homogeneity and high in-line transmittance. The in-line transmittance of a fabricated $Yb:Y_2O_3$ laser ceramic in the wavelength range from 400 nm to 6μmis shown in Fig. 1. High power high efficiency laser operations of the fabricated laser ceramics at 1.0μm, 2.1μm, and 2.7μm have been successfully demonstrated, respectively. Potential applications of Y2O3 transparent ceramics for laser oscillations in the visible and > 3.0μm wavelengths are also explored.

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Interatomic interactions in multilayer nanostructures based on the amorphous CoFeB alloy

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We analyzed interatomic interactions in two amorphous multilayer nanostructures (MLNS) $[(CoFeB)_{60}C_{40}/SiO_2]_{200}$ and $[(CoFeB)_{34}(SiO_2)_{66}/C]_{46}$, obtained by the ion-beam sputtering in the argon atmosphere with different content of metal alloy and with the inverse location of the non-metallic phases C and SiO_2 in the metal-composite layers (~4 nm) or in non-metallic interlayers (~2 nm).

Based on the analysis of XPS and X-ray absorption spectra, it was found that in the metal-composite layers the chemical bonds prevailing at the interphase boundaries between the CoFeB metal clusters and the elements of the surrounding matrix, forming predominantly carbide or oxide shells depending on the C or SiO_2 matrix composition.

Quantitative fitting of the Fourier transforms for the Fourier transformed EXAFS signal from two MLNSs shows, that in $[(CoFeB)_{60}C_{40}/SiO_2]_{200}$ with carbon in metal-composite the Fe and Co atoms of metal clusters have coordination numbers comparable to each other (6.73 and 7.68). In another MLNS $[(CoFeB)_{34}(SiO_2)_{66}/C]_{46}$, in which carbon forms interlayers, and its place in metal-composite layers is taken by SiO_2, the number of atoms in the nearest environment of Co (6.71) close to the previous one, and the number of atoms in the environment of iron atoms (3.37) most two times less and, rather, is typical for compounds of iron with oxygen from the composite matrix in this MLNS. This lead to more noticeable violations of the planarity of the interface and the anisotropy of electromagnetic properties in this MLNS compared to the previous MLNS.

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Grafting of cellulose, microcrystalline cellulose via polycondensation with oligo(lactic acid) and its applications in poly(L-lactic acid) based composites preparation

Md. Hafezur Rahaman[1], Mohd. Maniruzzaman[1], Md. Sagor Hosen[2], Md. Masud Rana[3] and **Md. Anamul Haque[1]**

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Poly(L-lactic acid) (PLLA) is a biodegradable polyester derived from renewable resources and used for both medical and ecological purposes. However, PLLA is not utilized in some applications due to further requirements for high impact strength and thermal stability. Properties of PLLA can be enhanced by blending or composite preparation with α-cellulose and micro-crystalline cellulose (MCC). To increase the compatibility, oligo(L-lactic acid) (OLLA) grafted onto their surfaces by graft poly-condensation reaction in toluene at 130^{0}C under 380 mmHg. Para-toluene sulphonic acid (5 wt.%) and potassium persulfate (0.01 wt.%) were acted as catalyst and co-catalyst in this reaction. For OLLA synthesis, ring-opening polymerization of L-lactides were carried out in the presence of stannous octoate (0.03 wt.%) as the initiator with L-lactic acids as the co-initiator; at 140^{0}C. Grafting was observed by FTIR and SEM analysis. FTIR absorption at 1730.15 cm^{-1} may due to bond formation between hydroxyl groups of α-cellulose and OLLA and spotted area of SEM images confirmed grafting of OLLA onto α-cellulose and MCC surface. MCC shows better grafting than that of α-cellulose. The surface morphology and thermal properties of the composites were investigated by SEM, XRD and thermal analysis (TGA, DTA, and DTG). SEM images of composite shows homogeneous distribution of grafted α-cellulose and MCC. WAXD profiles indicate only homo crystallization occurs in the composites. The results show an adequate compatibility between grafted α-cellulose/MCC and PLLA. Maximum weight loss temperature, degradation temperature and melting temperature of the composites increases with increasing grafted α-cellulose/MCC up to 15%. TGA and DTA results are indicating that grafted α-cellulose/MCC can improve thermal properties of PLLA based composites. DTG analysis also supports TGA and DTA results. This composite may have biomedical (scaffold, wound dressing) and ecological (food packaging, one time cup, plate, glass) applications.

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Models of thin beams, plates and shells based on the moment theory of elasticity as continuous deformation models for nanomaterials

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The construction of continuous models for nanomaterials (graphene, nanotubes, etc) is currently one of the topical problems. It is assumed that in the interatomic interactions of graphene (as well as nanotubes) there exist force independent moment interactions. This is logical, otherwise, in case of out of plane deformation (also in case of deformation of nanotube) graphene would not be endowed with rigidity. In this respect, it is essential to construct an atomic discrete model of graphene (or of one-layered nanotube) where, besides force interactions, moment interactions are also taken into account. When the interatomic interactions of graphene (nanotube) are replaced by the beam system, it becomes essential to construct a model of thin beams based on the moment theory of elasticity, where the beam deformation subjects to the concept "shear plus free rotation."

The present paper demonstrates the construction of such a beam model. Further, by replacing the interatomic interactions of graphene by the constructed model, the discrete-continuous model of graphene is constructed. After, by passing the limit, continuous – moment model of graphene (both for its in plane and out of plane deformations) is constructed. The latter is represented by the model of a thin plate based on moment theory of elasticity. In the result, the constants of the moment theory of elasticity are determined.

Further, the paper demonstrates the construction of the general model of thin shells based on the moment theory of elasticity, where the shell deformation (similar to the deformation model of graphene as a plate) is subject to the concept "shear plus independent rotation". In specific cases this model can serve as a continuous-moment model for one-layered nanotubes. Based on the constructed two models for graphene and nanotube, specific applied problems on in-plane deformation and out-of-plane bending deformations of graphene, as well as problems on the deformation of nanotubes, are solved.

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In Situ TEM studies of catalysts using windowed gas cells

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Atomic-scale insights into the structure evolution of nanocatalysts under reaction conditions are critical for correlating their structure-properties relationship. Detailed information at atomic scale, obtained by in situ TEM is therefore an essential complement to other in situ techniques (e.g., XPS, FTIR, etc.). In this talk, we present our in situ TEM studies of two nanocatalyst systems: (1) the CO-induced Pt nanoparticle surface reconstruction at saturation coverage (2) the facet-dependent oxidation of Pt_3Co ORR catalysts.

Atomic-scale insights into how supported metal nanoparticles catalyze chemical reactions are critical for the optimization of chemical conversion processes. It is well-known that different geometric configurations of surface atoms on supported metal nanoparticles have different catalytic reactivity and that the adsorption of reactive species can cause reconstruction of metal surfaces. Here, we characterize atomic-scale details associated with the structural rearrangement of supported Pt nanoparticle surfaces induced by the adsorption of CO at saturation coverage and elevated temperature. It was observed that the truncated octahedron shape adopted by bare Pt nanoparticles undergoes a reversible, facet-specific reconstruction due to CO adsorption, where flat {100} facets roughen into vicinal stepped high Miller index facets, while flat {111} facets remain intact.

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Microstructure based computational fatigue life prediction of structural materials

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Conventionally, engineers have to perform fatigue testing, either in stress or in strain controlled mode, to determine the fatigue properties of a material, which costs a great deal of time and money. Therefore, the concept of computational fatigue design has been proposed and received an increasing interest in recent years. In this research, a microstructure-based computational fatigue design model, named TMW model, is further studied by first using it to predict the fatigue crack nucleation lives of eight different alloys and steels, and comparing the predicted lives with that calculated values from the Coffin-Manson-Basquin relations which are obtained from experimental data fitting, second by developing the mathematical expressions of the surface roughness factor in the TMW model in terms of the arithmetical mean deviation of the assessed profile which can be determined experimentally, thus making the TMW model more applicable. In addition, a microstructure-based finite element analysis (FEA) model is created to investigate the effect of microstructural inhomogeneity (grain orientation) on the fatigue crack nucleation life of nickel-based alloy Haynes 282 in different strain ranges from Low cycle fatigue (LCF) to High cycle fatigue (HCF) at different stress amplitudes. Grain orientations are randomly assigned to a material representative volume element (RVE) with 20 random functions created for both HCF and LCF simulations. The TMW model shows effective for predicting the fatigue crack nucleation life of structural materials. The FEA simulation reveals that potential fatigue crack nucleation sites are likely to occur at grain boundaries right on or close to the free surface of the RVE. For both HCF and LCF cases, the simulated fatigue crack nucleation in Haynes 282 is more likely to occur in the grains of [1^{-}1 1] family, while the grains with the least probability of fatigue crack nucleation tend to be oriented towards [0 0 1] family.

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Model systems for heterogeneous catalysts at the atomic scale

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We have created model systems for heterogeneous catalysts on the basis of thin oxide films. This permits us to apply the toolbox of surface science for characterization and reaction studies at the atomic scale. Two case studies to demonstrate how those systems may be studied at the atomic scale are reported.

The first one discusses a novel characterization technique, namely surface action spectroscopy, using concepts developed in gas phase studies to record vibrational spectra of extremely dilute specimen based on messenger desorption. We demonstrate the extreme surface sensitivity of this technique by applying it to surface states of oxide surfaces, i.e. vanadia as well as iron oxides.

The second case study deals with a reaction in confined space using a model system based on a thin silica film, which is only bound to a metal substrate by dispersive forces, leaving a space between the oxide film and the metal substrate. Here we study water formation from intercalated oxygen, adsorbed on the metal surface and hydrogen provided from the gas phase in operando, and deduce the details of the kinetics of the reaction in confined space in direct comparison to the equivalent open space reaction. To this end we use a spectro-microscope, operated at BESSYII and developed in the group, which allows to observe tempo-spatial distribution of reactants and deduce apparent activation energies. Those experimental observations are interpreted on the basis of DFT calculations and kinetic models.

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Fully integrated microfluidic device transfigured from conventional 96-well ELISA kit

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ELISA using 96-well microplate has been widely used as a standard clinical diagnostics method, but it requires expensive materials with prolonged incubation time. In this work, a fully integrated active microfluidic device employing a conventional 96-well kit was implemented to improve the performance of traditional enzyme-linked immunosorbent assay (ELISA). The programmable and disposable on-chip pump and valve of the device precisely regulated a reaction time using optimized reagent volume to execute ELISA with consumption of reduced sample and reagents shortening the assay time, which are crucial for conventional ELISA using 96-well microplate. This unconventional device was successfully applied for the detection of cardiac troponin I (cTnI) of 4.88 pg/mL using minimum sample volume of 30 µL with shorter assay time of 15 min for each ELISA step.

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Thermoluminescence materials: Preparation techniques, perspectives and applications

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Luminescent materials have been successfully applied in diverse fields, which have greatly enhanced human life. Thermoluminescence (TL) is the emission of light upon heating a luminescent material after absorbing energy from ionizing radiation. The released energy, in the form of luminescence, and the sensitivity of photon detection makes the TL phenomenon an attractive method to measure small quantities of stored energy. Applications of the TL phenomenon are found not only in dosimetry, research, earth sciences, and age determination of archaeological or geological samples, but also for light-emitting diodes for home lightning, and bio-imaging medicine for cancer cells mapping. The preparation method of the TL material is critical because it controls the final characteristics, and hence the type of applications. The preparation method depends on the physical form required for the TL material, either polycrystalline powder, single crystals, or thin films. The most commonly used methods are precipitation and evaporation for the first, while Czochralski, zone melting, and precipitation from solutions or molten phases (flow method) for the second. For the thin films, the chemical vapor deposition, spray pyrolysis, and sol-gel are the typical techniques. A brief description of the preparation techniques, the analysis methods of the TL curves from the material, and the TL materials applications will be discussed in the conference.

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Novel application of fluorescent nanodiamond (FNDP) for infectious viral antigens: A rapid detection test for ebola virus glycoprotein

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Background and objectives: There is dire need for rapid diagnostic tests of high sensitivity, efficiencyand point-of-test reporting capability to mitigate lethal viral epidemic outbreaks. Our objective was to replace the contemporary colorimetric (visual) LFA (Lateral Flow Assay) for Ebola virus (EBV) by a new operating system that operate by Near Infra-Red (NIR) emitted from Fluorescent Nanodiamonds-NV-z~200nm (FNDP-NV-200nm)deposited on test line within the lateral flow assay (LFA) format. The objective was to gain unprecedented superior sensitivity, speed, quantitativedata, and high throughput capacity. Specifically, we aimed to detail technical issues and feasibility of deploying the new near infra-red operating system (OS) based on FNDP-NV-200nm.

Methods: FNDP-NV-200nm, 400nm or 800nm were linked to non-redundant anti-EBOV glycoprotein(GP) monoclonal antibodies (mAb) and tested for LFA performance by monitoring NIRemissions using an in vivo imaging system (IVIS) or an Opto-Electronic device (OED). Anti-EBOV glycoprotein (GP) humanized monoclonal antibody (mAb) c13C6 was linked to FNDP-NV-200nm forthe mobile phaseand a second, non-redundant anti-GP mouse mAb, 6D8, was printed on NCM at the Test-line. Goat anti-human IgG (GAH-IgG) served as a nonspecific antibody for capture of conjugatedFNDP-NV-200nm at the control line. Particles migration across the NCM in response to a fluidic pulse were assessed by NIR monitoring by an in vivo imaging system (IVIS).

Results: FNDP-NV-200nm-c13C6 specifically and dose-dependently bound to recombinant EBOV GP in vitro and was effectively captured in a sandwich configuration at the Test line by mAb 6D8. FNDP-NV-200nm-c13C6 was captured on the control line by GAH-IgG. The OED quantitative analysis of NIR (obtained in less than 1 minute) was further validated byIVIS.

Conclusion: FNDP-NV-200nm performance as a reporter for EBOV GP rapid diagnostic tests suggested an opportunity to replace contemporary colorimetric visual tests for EBOV GP and likely otherhighly lethal viral pathogens. Mobile, battery-operated OED adds portability, "Point of Need" (PoN) utility along with unprecedented speed, large volume of tests along with data transmission from PoN to authorities. Our data justify further development of the FNDP-NV-200nm OS and validation by authentic human specimens obtained from patients.

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Mechanochemical wear of silicate glass: Beyond the conventional materials removal

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Understanding the friction and wear of oxide glass is of great importance for its manufacturing and operation processes. Previously, it was indicated that the friction and wear behavior of oxide glass was very sensitive to the presence of water; due to the water induced mechanochemical reactions at glass interfaces can dramatically affect wear behaviors of oxide glass. However, when the wear track is formed by the water-induced mechanochemical process, the glass structure underneath the wear track may be affected by the shear stress along the sliding direction. With various experiments and Reax-FF MD simulations, it is found that when the glass surface is scratched with stainless steel ball in liquid water, the subsurface densification underneath the wear track of glass can occur during the mechanochemical wear process even though the contact load is lower than the indentation damage threshold of the glass. This is supported by that the wear tracks becomes hallower than the pristine wear track after the subsequent sub-Tg annealing, the enhanced nano indentation hardness and modulus, enhanced dissolution in the basic solution, and the change of the subsurface Si-O-Si bond angle and Si-O bond length distributions after friction tests and subsequent annealing treatment revealed by Reax FF-MD simulations. Therefore, not only mechanochemical wear induced material removal, the friction-induced subsurface deformation can also play important roles during the wear process of oxide glass.

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Impact of heated six constant Jeffreys model in a channel

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In the present investigation impact of heated six constant Jeffreys model of fluid on peristaltic flow in a channel is discussed in detail. Firstly, the modelling of the six constant Jeffreys model of fluid in two dimensional is presented. The complicated equations are simplified under the assumptions of long wavelength and low Reynolds number approximation. The highly nonlinear equations are solved analytically and numerically. Finally, graphical results are displayed to see the effects of various emerging parameters.

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Temperature noncritical processes in nonlinear and electrooptical crystals of mm2 symmetry group

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Temperature insensitivity of optical processes used in high average power laser systems is rather important problem that needs to be solved for a number of applications. Use of external thermal stabilization systems is not always effective and acceptable due to dimensions, weight or transit-time limitations. Besides, it is practically difficult or impossible to compensate powerful beam propagation channel local overheating caused by linear or multiphoton absorption in the crystal volume. In general temperature-noncritical (TNC) interactions in crystals are realized in the direction where the first-order temperature derivative of the refractive index is equal to zero. When this condition is satisfied simultaneously with the phase-matching condition for chosen frequency converter the corresponding TNC harmonic generation process might be realized. This work is focused on theoretical analysis and experimental study of the temperature noncritical frequency conversion in the nonlinear crystals of mm2 group and temperature not sensitive electro-optic modulation in E-O crystals of the same group. The possibilities of broadband TNC operation for the most promising representatives of mm2 crystal group have been demonstrated both numerically and experimentally.

In our experiments with frequency converters the positive wing of temperature range for second harmonic generation (1064 to 532 nm) in KTP ($KTiOPO_4$) crystal increased from 25°C/cm for the conventional cut to 210°C/cm for TNC cut. The corresponding temperature bandwidth for the third harmonic conversion in LBO($LaBaO_3$) crystal (1064 and 532 nm to 355 nm) changed from 3°C for the conventional cut to the 130°C for TNC cut. The reached conversion efficiencies under saturation conditions (two-pass schemes) were measured to be close to the case of the conventional cut utilization.

Widely used E-O Q-switches based on the KTP, RTP and RKTP crystals usually have dual-crystal design to compensate the dependence of a crystal birefringence on ambient temperature. Introducing of temperature gradients in the crystals affects dramatically on the Pockels Cells contrast. In some important applications the TNC cut for the crystals allows use of a single-crystal Pockels Cell design with stable performance in a wide range of the E-O crystals internal and ambient temperatures instead of using duel-crystal design.

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DFT+U-D3 study on the thermodynamics and modulation mechanism of H_2O and CO_2 adsorption on PuO_2 surface

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The adsorption thermodynamics and modulation of active molecules on PuO_2 surface are very important for the long-term storage of Pu. Within DFT+U-D3 scheme, a comparative study is performed to investigate the adsorption mechanisms, morphology, and phase diagrams of H_2O and CO_2 on PuO_2 (111) surface. Unlike the multilayer BET model of H_2O adsorption, CO_2 adsorption accords with monolayer Freundlich model as revealed by the calculated isotherms. The different adsorption behaviors are mainly due to the hydrogen bonds and Coulomb interactions between the adsorbed molecules. The hydrogen bonds promote the polymolecular adsorption of H_2O and the further partial dissociation at high coverage. The Coulomb attractive force among H_2O is larger than CO_2 and the attractive force among CO_2 rapidly decreases as the coverage increases. We clarifies the adsorption behaviors of H_2O and CO_2 and it could provide some important insights into the prediction of the surface corrosion reactions of PuO_2 in storage containers. The polarons induced by interactions between excess charges and lattice distortions play an important role in PuO_2 surface chemistry. Our result reveals that surface and subsurface electron/hole polarons play different roles to H_2O and CO_2 adsorption. Surface polarons can promote H_2O and CO_2 adsorptions. It is interesting that the subsurface electron polarons can promote H_2O adsorption but impede CO_2 adsorption, whereas the subsurface hole polarons just play the opposite role. Base on the comparative analysis of the chemisorption properties of H_2O and CO_2 and the electronic structures of the polarons, we put forward the inverse modulation mechanism by subsurface electron and hole polarons on H_2O and CO_2 adsorption, which can be used to manipulate the active molecules' chemisorption on oxides surface.

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Thermal, chemical and physical properties of Ethiopian Eri and mulberry silk fibers

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Silk fibre has received attention in the biomedical sector rather than textile production because of its excellent biocompatibility properties in the past century. Although silk fibre properties are different from area to area, it has created an opportunity in the biomedical sector to develop new silk-based medical textile products. This research work aimed to study the structural, physical, mechanical, chemical and thermal properties of Ethiopian silkworm cocoon's filament. Eri and mulberry silk fibre properties such as morphological structure, chemical properties, linear density, filament length, tensile strength, elongation, thermal property, and lustre were measured using ES ISO and ASTM standard methods. As statistical analysis result showed that eri silk fibre from Arba Minch had water removal temperature between 100℃ and 125℃ with degradation temperature of around 400℃ and eri silk fibre from both Addis Ababa and Awassa had almost similar water removal temperature around 100℃ and degradation temperature around 420℃. Tensile strength and elongation of both eri and mulberry silk fibre had significant differences among each region. The highest tensile strength of 4.47 cN observed from Addis Ababa, and the highest elongation of 20.01% found from Arba Minch eri silk fibre. The coarser linear density of 2.496 dtex from Arba Minch and finer count 2.392 dtex exhibited from Awassa. Arba Minch eri silk fibre had the highest filament length of 403.04 m and the least fibre length of 399.2 m recorded at Addis Ababa, and better whiteness (Rd) value of 58.21 observed at Arba Minch eri silk fibre. Bivoltine and multivoltine mulberry silk fibre had an average tensile strength of 8.01 and 11.83 cN, elongation of 10.3 and 12.1%, fineness of 3.2, and 3.16 dtex, filament length of 1208.6 and 1028.26 m respectively in the same place of Arba Minch. The morphological structure of eri silk fibre from each region had an almost smooth and clean surface, but bivoltine and multivoltine mulberry silk fibre was somehow rough and spots. According to the comparison results, Ethiopian silk fibres can be utilised more in the biomedical application and competitive in the global market.

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Design and fabrication of $SiC/IrSi_3$ composites for use in highly oxidizing environments

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Currently, MMCs with SiC as reinforcement emerge as ideal candidates for long-term stable devices withstanding high temperatures and harsh operating environments which are typical for many industrial sectors, such as energy, aerospace, electronics, catalysis, etc. However, the costly manufacture of such composites is the major restraint to make them marketable. In this paper, the design and fabrication of highly-dense, nearly-shaped $SiC/IrSi_3$ composites, effortless produced at T = 1250°C under a vacuum by reactive melt infiltration of liquid Si-62 wt%Ir eutectic alloy into bimodal SiC_p-C porous preforms, are presented. The replacement of unreacted detrimental Si by a tougher and less oxidizing intermetallic phase ($IrSi_3$) was successfully obtained. As it will be introduced during the talk, the know-how gained from preliminary fundamental studies performed on liquid Si-Ir thermo physical properties, thermodynamic properties of Si-Ir-C, as well as on the reactivity at the liquid Si-rich Si-Ir alloys/C and Si-Ir alloys/SiC interfaces, was crucial for optimizing the reactive infiltration process. Finally, a high compatibility of $IrSi_3$- silicide with SiC and an improved oxidation resistance of the SiC-Si based composites by the presence of the Ir-silicide phase were observed during thermo-mechanical characterization, as expected.

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Stimulation analysis of aircraft wing skin panel using laminate lay-ups

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The main objective of the research work is to eliminate divergence of swept wing by using proper fibre angle orientation of composite material with better mechanical properties. It is mainly done by aeroelastic tailoring using composite material. Basically, the wing behaviour of an aircraft is characterized by the interaction between the material and shape of the wing. The forward swept wings prove to have high aerodynamic efficiency, if the divergence problem is eliminated. These forward swept wing aircraft is one of the most superior aircraft in terms of both aerodynamics and structural configurations. This design has been consistently frustrated by the divergence problem. Generally, in the forward swept wing, when the aircraft turns, it applies high G-loads on the wing, this load causes the wing tip to bend upward which in turn leads the twist of the leading edges in the upwards direction. This bending is known as divergence, which increases the angle of attack leading to failure of wing. More over the divergence in the wing can be reduced by increasing the wing bending stiffness which in turn associates with the increase in the weight of the wing that leads to increase in overall weight of the aircraft. This weight penalty is known to be very severe for conventional metal wings, but with the unique lightweight property of advanced composites the designer will be able to overcome the difficulty in designing. Fibre angle orientation means the individual arrangement of the fibre in the development of material. As it greatly influences the property of the material, we chose this as a prominent key to avoid divergence. The materials involved in this research works are Glass fibre, Glass epoxy and Kevlar epoxy. The simulation and mathematical calculations of these materials are conducted by using MSC NASTRAN and MATLAB. Finally, comparison of mathematical and simulation works provides a better results for elimination of the divergence problem.

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The physical chemistry of steel deoxidation and nozzle clogging in continuous casting

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Nozzle clogging in continuous casting of steel originates by the adherence of alumina particles and other oxides, precipitated during the liquid steel deoxidation, on the refractory nozzle material's surface. Hence, these particles' nucleation and growth rates in supersaturated melts are analyzed considering, specifically, the role of the interfacial tensions between alumina, silica, and other oxides and the liquid metal. Weak steel deoxidizers like silicon do not need high super saturations favoring high nucleation rates, giving particles' narrow size distributions thanks to fast diffusion and Ostwald-ripening coagulation. Strong deoxidizers, like aluminum, need high super saturation levels leading to broad size distributions. Besides, the morphology of these particles depends on the nucleation and growth mechanisms. The adhesion forces among the deoxidation particles, forming clusters, depend on the morphology and the oxide's chemistry. The stability of the nozzle's clog, adhered to the nozzle's wall, depends on the interface tensions between the melt and the nozzle's refractory surface and between the melt and the inclusion. The results obtained here help set up basic recommendations in steel refining and materials specifications of casting nozzles. The effects of the nozzle material on the clogging intensity and its effect on fluid flow dynamics of liquid steel inside the slab mold is simulated using Computer Fluid Dynamics techniques.

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Synthesis and characterizations of MPS/PANI heterojunctions doped with erbium

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P-type silicon was used for the formation of macroporous silicon (MPS) by electrochemical corrosion in HF:DMF solution, 1:9 in volume. The Schottky structure was obtained by depositing polyaniline (PANI); which was doped with different contents of erbium (Er) using cyclic voltammetry method, in millimolar order (mM). The structural analysis by scanning electron microscopy (SEM) showed that the pores are formed randomly throughout the porous region, with diameters ranging between 0.25 and 1.20 µm and length around 15 µm. The Spectrometry analysis X-rays by energy dispersion (EDS) reveals that the PANI was deposited along the pore walls, with a higher concentration in the regions closest to the surface. Rutherford backscattering spectrometry (RBS) shows that Er has been diffusing through the PANI layer, but with greater concentration at the superficial region. According to the Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) analysis, the presence of Er gave rise to the formation of additional functional groups besides that corresponding to polyaniline and silicon oxide phases. In samples doped with Er, both FTIR and Raman spectroscopy showed that Er creates additional functional groups that, according to X-ray diffraction (XRD), reduce the crystallinity of PANI and with that decrease the conductivity. The electrical characterization confirms not only the decrease in the conductivity of the PANI but also the decrease in the current that passes through the MPS/PANI junction. Those are associated with the increase of the SiO_2 within the porous structure. This effect was partially recovered by the inclusion of Er, possibly due to its effect of reducing the width of the space charge region. The effect of Er present in the MPS/PANI interface through the modification of the work function or the increase of surface states.

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Effect of adding Ta and W monocrystalline fibers in Ta-metallic glass matrix using molecular dynamics simulations

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In this work, we study the effect of adding Ta and W monocrystalline fibers in Ta-metallic glass (MG) matrix using MD simulations with the embedded atom method (EAM) to describe the interatomic interactions. In addition, mechanical solicitations have been performed using a tensile test under a strain rate of $10^7 s^{-1}$, the evolutions of stress-strain curves have been compared between four samples (Ta-MG, nanoporous Ta-MG, monocrystalline Ta-reinforced Ta-MG, and monocrystalline W-reinforced Ta-MG). Tensile tests have shown that plastic deformations are characterized by the localization of shear bands (SBs) in amorphous zones and the addition of Ta monocrystalline fibers increases the ductility of the material and decreases its ultimate tensile stress (UTS); this ductility was found to be a result of the crystal growth inside the glassy matrix triggered by the crystal phase of the fiber. In contrast, the addition of W reinforces the MG matrix and increases the maximum strength and the toughness of the material, this improvement of the mechanical properties was explained by the presence of the heterogeneous interface which behaves as an obstacle to the motion of shear bands.

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Photostability and beam strength of polyurethane matrices for active element of solid-state dye lasers

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Among the main requirements, which should be met by the polymer matrices in dye laser solid-state elements, their photostability and beam strength are crucial factors. Here photostability is understood as polymer resistance to photo oxidation and photochemical destruction, and beam strength means ability of the material to withstand irreversible changes of its optical parameters and retain integrity under strong optical irradiation (in particular, by a laser), including stability to local overheating. The use of polymer matrices based on polyurethane elastomers allows providing stable operation of dye lasers due to high segmental mobility and effective control of properties using different components and various curing conditions.

Effect of variation of diisocyanate and glycol polyurethane components on photostability and beam strength of the polyurethane matrix have been investigated as well as the methods of that characteristics evaluation. This work presents a comparative analysis of photo oxidation destruction characteristics for different PU polymers, and their beam strength parameters, obtained by various methods (IR-spectroscopy, dynamic mechanical analysis (DMA), paramagnetic probe and laser experiments).

Elastic characteristics in a wide temperature range and high beam strength of the obtained polyurethanes cause prospects of these materials for the applications as efficient solid-state laser elements. The observed good agreement in the correlations between the polyurethane chemical structure and changes in the modulus of elasticity, probe relative penetrability, probe correlation time, amount of OH-containing radicals formed after irradiation, and also the measured values of the single-pulse laser damage threshold, allows to predict stability of further developed polyurethane-based materials under continuous laser operation.

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Fractographic investigation of interfacial bonding of typha fiber reinforced epoxy composite

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Natural fibers have poor bonding compatibility with the polymer matrix, so it is necessary to conduct the chemical treatment. One of the most used treatments for the modification of natural fiber was the alkali treatment. Alkali treatment conducted to improve the compatibility of the bonds between the fibers and the matrix. This work aims to investigate the interfacial bonding between Typha fiber and epoxy matrix after going through impact testing. Untreated and alkali-treated fibers are prepared before being fabricated into composites. The fibers are immersed in a 5% NaOH solution for 1.The SEM observations revealed that the debonding fiber from the matrix is one of the main causes of the damage on composite and alkali-treated fiber has a stronger bonding condition than the untreated fiber. The rougher the fiber surface will be the better the interlocking mechanism of fibers and matrices. Alkali treatment plays important role in changing the roughness of the fiber surface. The untreated Typha fiber-reinforced epoxy composite occurs a lot of dislocation between the fibers and the matrix, which is many fibers are no longer embedded in the matrix, this phenomenon indicates that the composite has severe debonding and fibers pull-outs. Therefore, we can conclude that the alkali treatment process on Typha fiber has succeeded in improving the bonding mechanism of Typha fiber and epoxy matrix.

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Effect of nano-scale graphene and carbon nanotubes on mechanical properties of alumina- zirconia nanocomposites

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The brittle nature of alumina and other technical ceramics limits their mechanical performance under various operating conditions. Through microstructural tailoring, the fracture toughness and other mechanical attributes of alumina can be improved adding nanoscale materials such as graphene, carbon nanotubes and zirconia to form a nanocomposite. For the current studies, alumina-zirconia nanocomposites reinforced with both graphene and carbon nanotubes have been fabricated via colloidal mixing and followed by hot-pressing sintering process. The effect of 0.5wt% graphene and 2wt% carbon nanotubes on the alumina-zirconia microstructure and mechanical properties were characterized using the single edge notched beam (SENB) test and conventional indentation fracture toughness (IFT) test. Typically, there is a relatively high degree of grain refinement of the nanocomposites due to the synergistic effect of carbon nanotubes and graphene. This directly influenced the physical and mechanical properties of the hybrid nanocomposites such as density, hardness and fracture toughness. Fractography studies after the SENB tests also demonstrate the toughening mechanisms of the individual carbon additives as well as their synergistic role in improving the fracture toughness of monolithic alumina. Both intergranular and transgranular fracture modes were depicted by the hybrid nanocomposites during the bending tests are were prevalent in the fractography of the fabricated samples.

Nonlocal approach to energy bands in periodic lattices and emergence of electron mass enhancement

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It is well-known that quantum states of light and matter are basically nonlocal which reflect the fundamental property of wave-particle duality. Nonlocality which is the most fascinating and hardly understood phenomenon of the quantum theory is in general manifested when measurements (in space or in time) on two or additional isolated quantum mechanical systems are achieved. As a result, physical effects can be correlated technically to some extent defying any local classical explanation and for that reason quantum mechanics is nonlocal. It was argued in that an association between Heisenberg's uncertainty principle (HUP) and non locality holds for merely all physical systems and moreover a link between the "Einstein's spooky action at a distance" concept and HUP exits. We analyze energy bands in periodic lattices based on the nonlocal-in-time kinetic energy approach. We consider the electron dynamics in the periodic potential and construct a nonlocal approach to the weak binding case in three dimensions. A number of features are revealed. In particular, we demonstrate an effective mass enhancement for electrons of around $m^{*} \approx 1.67\alpha^{-1}\ \mathrm{GeV}$ for typical solids, where is a real free parameter.

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Progress of nanotechnology in industrial applications: Advanced strategies with innovative nanoparticles

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Nanotechnology has received substantial attention since the concept of dispersing nanoparticles into a base fluid was first introduced in the later part of the 20th century. This is evident from the increased number of investigations and pilot experiments related to this field. The in-deep attention to its resulting fluids (a-k-a nanofluids) is primarily due to their enhanced thermophysical properties alongside their ability to be incorporated into a wide range of industrial applications. Therewith, and despite the benefits of this innovative technology, there is a need for a holistic review of the strategies and steps concerning their application in various devices. This should be provided from the preparation process of nanoscale particles (e.g., pilot-synthesis, characterization, and stability measurements) to the applied boundary conditions, which remains a difficult challenge. Sequence to this, our oral presentation aims to update researchers on the recent progress of this technology while highlighting the challenges and the future of advanced strategies for the next-generation of industrial devices, such as solar collectors, heat exchangers, refrigeration systems, radiators, and storage systems. A summary of the merits and demerits of this advanced technology will be deeply discussed besides some recommendations of experts for future investigations. This would broaden the open literature and applicability of these strategies in the industry of tomorrow.

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Behavior of molar volume evolution in time of ZnO zinc blend type under different temperatures and pressures a molecula dynamics computation

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In order to analyse the behavior of molar volume evolution in time of ZnO rocksalt structure under extended pressure and temperature; we investigate parallel molecular dynamics and DL_Poly_4 software on RAAVEN supercomputer of Cardiff University (UK). We use the range of temperature 300-3000K and 0-100GPa for 5832 atoms of ZnO. The interatomic interactions are modeled by Buckingham-Coulomb potential. Although no more data available under previous conditions, our work is in vicinity of theoretical and experimental information. These results have great importance especially in Nanotechnology.

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Effect of recycled coarse aggregate on physical and mechanical properties of concrete

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Recycling of building waste has become essential process in the construction industry due to the sustainability and economic benefits such as decreasing the waste to landfill, conserving natural resources, and reducing pollution. Large amount of building waste is produced from the construction and demolition process of reinforced concrete (RC) structures. In this paper, the effect of using recycled coarse aggregate (RCA) on the behavior of concrete is experimentally studied. The RCA is prepared by crushing and sieving of waste of standard compression test cubes having a compressive strength ranging between 25 MPa and 30 MPa. The physical and mechanical properties of RCA are experimentally estimated and compared to those of natural coarse aggregate (NCA). A set of 72 standard concrete cubes, cylinders, and beams specimens are made using coarse aggregate replacement ratios (CARR) of 0%, 30%, 50%, and 100%. The specimens are tested to estimate the compressive, splitting, and flexure strengthens at the ages of 7 and 28 days. The study is extended by using the RCA in casting 12 RC columns with CARR similar to those of specimens. The columns are tested in an axial compression test protocol till failure. Crack patterns, failure loads, strains, displacements, and toughness of the tested columns are compared. Also, tensile strength, modulus of elasticity, and fracture energy of the plain concrete specimens are investigated. It is concluded that using a CARR of 30% and 50% and a specific water cement ratio provides better mechanical behavior than that of NCA while the CARR of 100% yields worst mechanical behavior compared to that of NCA. The obtained conclusions are valid provided that the properties of the source concrete used in the recycling process are controlled.

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Effect of hybridisation on the acoustic response of composite laminate for prefabricated building construction

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The reduction of environmental impact (carbon and energy footprints) of building construction is increasingly becoming important. Prefabricated building construction which involves having modularized components of a building fabricated offsite in a manufacturing facility for rapid assembly onsite provides a solution to this challenge. Beyond process efficiency and cost saving gains, prefabricated building construction creates a myriad of environmental benefits, such as reduction in energy use for construction, reduction in material waste, support for adaptation-reuse-and-recycling, amongst others. Sandwich panels find application in buildings as partition/external walls and roofing panels, due to their lightweight, inherent thermal insulating characteristic and adaptable acoustic response. The construction of these sandwich panels consist of an inner and outer thin skins made from either galvanized steel, stainless steel, aluminum or glass fibre reinforced polymer (FRP). These materials are separated by a core made from either polyurethane (PU), polyisocyanurate (PIR) or rock wool, depending on functional needs: structural, thermal, acoustic and vibration behaviours, amongst others. There is need to further improve their required properties, which include lightweight, sustainability, and environmentally friendliness, in addition to the aforementioned main functional properties of buildings. Therefore, this paper investigates into the acoustic response of a hybrid sustainable composite for sandwich panel material. Test samples consisted of different volume fractions of hybrid glass/flax fibre in epoxy resin matrix system. For each set of the test samples, acoustic properties (mainly sound absorption coefficient and transmission loss) were determined based on ASTM E1050 standard, considering a plane wave impedance tube equipped with two microphones spaced at a known distance apart, and at a given distance from the test sample.

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Advancing the a posteriori quest for deep-blue phosphorescence

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To advance the a posteriori quest for deep-blue phosphorescence, we quantify the degree of metal-to-ligand charge transfer (MLCT) upon excitation using density functional theory calculations. We also comprehensively determine how the MLCT nature of a state is correlated with the wavelength of potential phosphorescence through comparing the results of two typical ligand structures, i.e., 2-phenylpyridine and 1-phenyl-3-methylimidazolin-2-ylidene, with those of their derivatives. The MLCT nature can be defined as the difference in the electron density over the central metal ion that contributes to the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO, respectively). This study focuses on how the MLCT nature can be characterized upon excitation depending on the admixtures of molecular orbitals and how a stronger MLCT nature is preferable for efficient phosphorescence, while the MLCT nature exhibits a trade-off relationship with the wavelengths of phosphorescence in the blue region. Moreover, we elucidate how iridium(III) complexes are suitable for efficient phosphorescence and discuss a conceptual grand design for transition-metal complexes with deep-blue phosphorescence using the ligand field theory. We examine why strong MLCT nature upon excitation does not necessarily ensure highly efficient phosphorescence, taking into account possible relative energy gaps between the singlet MLCT, triplet locally excited, and d–d transition states in a transition-metal complex formed after excitation. Nevertheless, the initial MLCT serves as a necessary condition that induces corollary energy-state configurations as well as decay from the excited states. Therefore, quantifying the nature of that MLCT, which is the first process upon excitation, with the possible wavelength of phosphorescence, is a useful parameter for a conceptual grand design for candidate complexes that can efficiently emit deep-blue phosphorescence. This reverse method of analyzing candidate complexes before experimentally formulating and studying them can accelerate the a posteriori quest for deep-blue-emitting materials.

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Parametric optimization for aerospace quality holes using helical milling

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The optimized process parameters in helical milling of CFRP/Ti-6AL-4V stacks are evaluated to achieve H7 or better holes with minimum tool wear. Eccentricity, spindle speeds, helical pitch, tangential feed and nanoparticles lubricant are selected as input parameters while the machining performance is measured in terms of tool wear, holes accuracy and surface integrity (Surface Roughness, Burr Height). For better lubrication and environmental friendly machining, a MQL system is used. Results show that spindle speeds of 7500 rpm for CFRP, 1000 for Ti-6Al-4V, eccentricity of 2mm, 1mm pitch, tangential feed of 0.01 and 1% MoS_2 resulted in more than 90% holes conforming to H6 standard with minimum tool wear.

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Advanced microscopic analysis of a Sri Lankan anthill clay variety for the investigation of industrially demanded characteristics

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Anthill clay is some sort of specific clay variety among other common clay types because of the mode of available in the Environment while obtaining some extraordinary characteristics when comparing with some other well-known clay varieties. According to the most outstanding research outcomes that related with the clays, there were discovered some advanced characteristics of some different anthill clay verities which are useful in the advanced industrial uses such as the refractory materials, adsorbents, catalytic activities and more advanced chemical processes. Sri Lanka is a country which is much rich in natural clay deposits. In the existing research there were expected to microscopically characterize a selected anthill clay variety for the sake of advanced industrial uses. The clay samples were collected nearby a known range of anthills from a specific region around Matale area. The dry powdered anthill clay samples were characterized using a Scanning Electron Microscope (SEM). The captured Scanning Electron Microscopic (SEM) images showed that the presence of kaolinite, illite, muscovite and montmorillonite as the major clay minerals in this anthill clay type with the silt coated conditions. When considering about the montmorillonite which is an important component of bentonite clay, it has been identified as a multi-purpose material in the manufacturing of cost effective eco-friendly fruit and vegetable containers, environmental pollution control material because of the adsorption capacity against some anions, cations, heavy metals and some toxic compounds that dissolved in water and air and also in the pharmaceutical and medical applications because of the adsorption capacity for some toxic and harmful substances while having less harmful conditions for the human skin. Therefore, this anthill clay variety can be further developed for some advanced industrial applications while identifying some extraordinary characteristics.

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Effect of surface treatment on fatigue of composite support wind turbine blade

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The cyclic deformation behavior of two metal-matrix composites, namely, aluminum-based composites reinforced with a steel wire and an aluminum alloy 3030 wire, were investigated at room temperature for wind blade support. All materials were synthesized using sand-casting and subjected to mechanical surface treatment using ball burnishing. High-cycle fatigue was observed under reversed bending-loading at 50 Hz. The composites reinforced with wire volume fractions (28% and 34%) show excellent fatigue life and endurance limits under stress-controlled conditions. The tensile and microstructural properties of these materials were also examined. The alloyed aluminum-matrix-steel-wire-reinforced composite showed higher fatigue behavior than the wire reinforced using ball burnishing of as-cast alloys.

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"The convergence of technologies, generates convergence in the regulations"

Guillermo Valdes Mesa
Havana University Center Biomaterial, Cuba

The convergence of nanotechnologies generates synergies among different technologies to say, nanotechnologies, neurotechnology, computers and biotechnology, these technologies must converge their regulations, the application of medical devices in nanotechnologies should lead us to a link between the technical committee TC 210 and ISO technical committee 229 link that does not exist in our work in this moment In this do an analysis of the management of risk from an optical NC-ISO 14971. Studying the global trend in this respect as imported for manufacturers medical Devices worldwide. The convergences of technologies is a consequence of atomic precision, where the boundary between the biotic and abiotic mute blur the interaction. The interaction between nanotechnologies, biotechnology and informatics and communications (NBI) generates a synergy of unusual consequences of all is known that the industry of semiconductors is the one of greater precision that is atomic, the new medical devices that will be applied in the teranocis will dose Physical principles that will be governed under the laws of quantum mechanics, but there are two problems that have not been solved even though they are one the non-existence of quantum biology and the transition from quantum to classical mechanics. On the other hand, the redefinition of the international system of units based on the universal constants that will be implemented by 2018 has a deficiency that is the second that redefirms implies redefinition of the meter the chain of traceability proposed for nanometrology presents a serious difficulty when putting the microcopy of atomic force wing of effect tunnel situation that is changing the verification of the Wiedemann-Franz law at atomic level yields a result where the phononic component is taken into account, a result that launches STM to the cusp of the chain of traceability above inclusive of interferometry.

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Role of phase superposition on the electrocaloric properties in Ba-based ceramics

L. Curecheriu, V.A. Lukacs, L. Padurariu, C.E. Ciomaga and **L. Mitoseriu**

Alexandru Ioan Cuza University, Romania

In the last years, there is a high interest in developing alternative cooling technologies because: (i) it is important to reduce greenhouse gases that are used heavily in domestic and industrial refrigeration; (ii) high current densities in integrated circuits impose higher demands on cooling systems that cannot met by the fan-based solutions. The main advantage of electrocaloric (EC) refrigeration is that by comparison with magnetocaloric solid-state refrigerators based on another solid-state cooling technology, the big-sized magnet is still a drawback. $BaTiO_3$(BT) family as EC materials has been studied quite extensively in the past several years in various forms including thin films, bulk ceramics (also multilayer ceramic capacitors -MLCC) and single crystals and a large ΔT has been reported for BT-ceramics in the vicinity of ferroelectric-paraelectric (FE-PE) (tetragonal-cubic T-C) phase transition. Owing to the high transition temperature the using of pure BT as EC materials is limited, but this can be properly modified by incorporation of suitable dopants.

In the present paper, we prepared and investigated $BaZr_xTi_{1-x}O_3$ ceramics with x=0.02; 0.04;0.06;0.08; 0.10;0.12;0.15; 0.175; 0.20. X-ray diffraction data showed the phase purity and SEM images demonstrated homogeneous microstructures (average grain size between 10-5 μm) and well-defined grain boundaries. Impedance spectroscopy in the temperature range of (25 to 150)°C shows a composition-induced ferroelectric-to-relaxor crossover with compositional-dependent shifts of the structural transition temperatures by comparison with ones of the pure BaTiO3.All samples are tunable, DC tunability increasing with x from 2.11 (x=0.08) towards 2.6 (x=0.20) at 25 kV/cm. Polarisation vs. E loops indicate regular variation with increasing Zr addition, a reducing of loop area, remanent and saturation polarization from P_{sat}=15μC/cm^2 to P_{sat}=9μC/cm^2 and increasing of loop tilting. EC effect was indirect evaluated from P(E) loops with temperature and a maximum of 0.7 K was obtained for x=0.04 at 373K.

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Phase superposition as origin of enhanced functional properties in $BaTiO_3$ - based ceramics

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The role of polymorph superpositions around room temperature in $BaTiO_3$ ceramics with grain size (GS) between 75÷2250 nm was investigated to check the GS-dependence of their structural and functional properties. Superposition of orthorhombic-tetragonal or of more polymorphs with variable amounts around room temperature are affected by size reduction and plays an important role, mostly on the properties measured after dc-poling (pyro/piezoelectric properties). Permittivity vs. dc field dependences shows field-induced structural transformations (slope modification) at dc fields ~10 kV/cm, which were confirmed by XRD analysis realized in remanence on poled ceramics.

The phase superposition around room temperature is a tool which can be exploited to enhance functional properties and is responsible with high permittivity, piezoelectric and pyroelectric constants in $BaTiO_3$-based ferroelectric ceramics. In porous $BaTiO_3$ ceramics with phase coexistence, low density favors the tetragonal state while high density promotes the stability of lower symmetry phases (orthorhombic, rhombohedral or both). For doped-$BaTiO_3$ ceramics, the high polarization and piezo/pyroelectric constants are reached when orthorhombic-tetragonal superposition is obtained around room temperature (for example, in 5% Sn additions). This is explained on the basis of thermodynamic models. A Landau-based calculation indicates the possibility of metastable polymorph states coexistence around room temperature. The phase composition may be altered by dc fields (field-induced structural transformations) and by the application of strain-stress fields produced by substitutions, structural point defects or dislocations. In conclusion, even in a classical well-known ferroelectric material as $BaTiO_3$, the coexistence of polymorphs may be induced in specific conditions and it can be used to enhance the properties.

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Novel approaches for strongly enhanced mechanical performance of bonded joints

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Current aerospace, automotive, and shipbuilding are pursuing the fabrication of strong and damage-tolerant components using advanced joining techniques. In that respect, adhesive bonding plays a crucial role because it eases the assembly process and provides increased design flexibility. Adhesive properties and morphology/topography of mating surfaces control the mechanical performances of the joints. Recent work has shown that substrate architecture represents a new scale for the joint design and allows us to tune deformation and fracture mechanisms, crafting layered structures with enhanced strength and toughness. Unprecedented developments in additive manufacturing are hastening this approach. This talk will support this point of view and leverage the results of the most recent research work on the analysis of deformation and fracture of layered materials. The presentation will showcase the results of the author and co-workers' ongoing collaborative efforts that focus on tailoring bond line and interfacial architectures to achieve enhanced mechanical behaviour. After that, I will dive into current research to unravel the existing interplay between adjoined layers' architecture and the resistance to interfacial separation. The discussion will be mainly framed into the latest experimental results that include 3D printing, fracture testing, high-resolution in-situ imaging of the fracture process. The talk will highlight that material architecture promotes a snap-through cracking process represented by a sequence of non-equilibrium transitions accompanied by sudden load drops and a local release of strain energy. The tantalizing opportunity of tuning energy dissipation by tailoring material architecture will be emphasized with the aid of design exploration and computational fracture mechanics.

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Structural, fatigue behaviour and mechanical properties of Zirconium Tungstate-reinforced casted A356 aluminium alloy

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The aim of this study is to investigate the structure–property relationship of the zirconium tungstate-reinforced casted A356 aluminium alloy. The reinforcement ceramic used was zirconium tungstate of the negative thermal coefficient type, which assists in the weldment of crack growth and enhances the fatigue life. The specimens used in this study were casted by stir casting method and prepared according to Compact Tension standard E-399, and microstructural, fatigue behaviour, and mechanical properties were investigated systematically. Microstructural analysis showed reduction in porosity by the addition of ZrW_2O_8 particles. Fatigue results depict the increase in the fatigue life of aluminium reinforced ceramic as compared to the casted base aluminium alloy. Brinell hardness of ZrW_2O_8 reinforced alloy samples increased 7% as compared to the base aluminium alloy hardness value. Tensile strength also significantly improved from 176 MPa for the base A356 alloy to 198 MPa for the ZrW_2O_8 reinforced composite. Furthermore, addition of ZrW_2O_8 ceramic powder increased the fatigue life more than 50% of the base alloy. These results suggest that the ZrW_2O_8 reinforced A356 composites may be potential candidates for aerospace industry, military, transportation and in structural sites.

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Chalcogenide filled nanoporous silica glass composite for photonics

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New composite material made from porous silica glass as low refractive index matrix and As_2S_3 chalcogenide glass in form of high refractive index nanoparticles filled in these pores is created and investigated as functional material for photonic applications. The fabrication method is based on preparation of chalcogenide nanoparticles in solvent and impregnation of porous glass matrix followed by heat treatment.

Functionality of such materials is provided by size-limited chalcogenide material, which possesses variable optical parameters (absorption, refractive index) based on reversible optical and structural transformations under active illumination or heat treatment in such chalcogenide-containing composite. These are compared with effects in simple As_2S_3 layers: the photodarkening- bleaching or erasing the optically recorded image can be repeated multiple times enabling reversibility of amplitude-phase optical relief as part of 3D element like optical waveguides, coupling elements.

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Geometric and optical properties of pits in CR-39 plastic etched after irradiation by 216 MeV/amu ^{12}C beam at different depths of water-chamber

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This work belongs to the direction of multilateral research of the system of the accelerated beam ^{12}C plus the CR-39 plastic detector. The use of a highly sensitive plastic detector, on the one hand, makes it possible to study the properties of the ion beam, on the other hand, it makes it possible to investigate the results of the action of the beam on the plastic detector itself. Both results are very important for numerous physical studies medical applications, but in addition to these studies, the second result allows changing the properties of surfaces and the internal structure of materials by irradiation with ions, which can be important for the field of Materials Science. Beam of 216 MeV/amu ^{12}C ions irradiated CR-39 plates in biochamber at the TWAC-ITEP accelerator. The plates were etched and dried. A system microscope-computer made about 50 scanned micrographs from each surface of eight plastic plates irradiated in different depths of biochamber filled by water (main experiment) and of one plate irradiated in the same biochamber but filled by air (auxiliary experiment).

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Enhancement of photoluminescence properties of nano-sized Pr^{3+} doped $LuPO_4$ powders by incorporating of Y^{3+} ions

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The work explores the enhancement of photoluminescence properties of nano-sized $LuPO_4:Pr^{3+}$ phosphor powders synthesized by sol gel process with incorporation of yttrium ions inside of this single matrix to obtain $(Lu_{1-x}Yx)PO_4$: Pr^{3+} (x=10, 20, 30, 40, 50 at. %) powders. Under UV excitation at 270 nm the emission spectra of $LuPO_4:Pr^{3+}$nanopowder do not present any characteristics emission band attributed to $4f^15d^1 \rightarrow 4f2$ transitions of Pr^{3+} ions, while a large emission band has been observed which due to defects created in $LuPO_4$ cell by doping considering the ionic radius of Pr^{3+} is larger compared to the ionic radius of Lu^{3+}, this band extinguishes gradually at the time insertion of the Y^{3+} ions until its total disappearance (for x=40 at. %).It was found that the emission spectra of $(Lu_{1-x}Y_x)PO_4:Pr^{3+}$ nanopowders under λ_{ex}=230nm presents only the characteristics emission bands of Pr^{3+} ions with a remarkable influence of the rate of Y^{3+} ions on the intensity of this bands. Furthermore, it was observed that the improvement in the luminescence properties of $(Lu_{1-x}Y_x)PO_4$: Pr^{3+} nanopowders is very remarkable in visible range.

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Biofuel production using ordered mesoporous carbons with modified carbonaceous structure

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Monometallic and bimetallic supported catalysts were developed to produce 2,5-dimethylfuran (DMF) trough hydrogenolysis of 5-(hydroxymethyl)furfural (HMF). Detailed physicochemical characterization was done in order to understand structure-activity correlation. Through a series of experiments and comparatives tests, the synergistic effect among Pt, Ir, and Ti incorporated in the support was investigated. Results revealed that using the titanium contained ordered mesoporous carbon, synthesized by a novel technique, high selectivity to DMF was achieved. In the case of the best catalyst PtIr-TiC, the good activity and excellent selectivity to the desired product DMF (98% yield) was related to the high hydrogenating capacity of the bimetallic sites, the acid support characteristics and the high metal nanoparticles dispersion achieved on the mesoporous titanium modified carbon support.

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Anisotropic multiscale modelling in SAE-AISI 1524 gas Tungsten arc welded joints

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A transient non-linear multiscale finite element heat flow-mechanical model to determine micro residual stresses (type III) and micro plastic strains in SAE-AISI 1524 gas tungsten arc welded joints is developed. To include anisotropy by preferred crystallographic orientation or texture, the global domain was decomposed into small sub domains based on the concept of representative volume elements (RVEs). A three-dimensional numerical procedure was developed by using the coupling DREAM. 3D-ABAQUS. The macro scale temperature gradient information as prescribed driven (load) boundary conditions was used to calculate the meso thermal cycles, and the meso scale temperature gradient information was used to calculate the micro thermal cycles needed in the subsequent mechanical analysis. Anisotropy was included by randomly entering in each grain of the RVE specimen either the maximum Young's modulus (Emax) in the stiffest direction, or the minimum Young's modulus (Emin) in the least stiff direction. Under this assumption, the averaging of the grain orientations over all grains in the textured polycrystal with greater number of grains ocurred, and the strength was diluted by the spread of orientations present. Higher Mises stresses evolved in the sample with coarse grain size (16 μm), which indicates that the strong dependence of residual micro stresses on grain size was reversed. The influence of the grain size on the response of the aggregates is clearly observed.

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Improvement in the carbonation resistance of construction mortar with cane bagasse fiber added

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In this work, sugarcane bagasse fiber, a waste product of agro industry, was added to mortar mixes at different proportions looking to seal porosities so as to improve the resistance of concrete to carbonation and to improve its mechanical properties. To evaluate the behavior of bagasse fibers in the alkaline media typical of mortars, bagasse fibers were subjected to solutions with alkaline pH values, and their chemical and morphological behavior was evaluated using FTIR (Fourier transform infrared spectroscopy) and SEM (Scanning Electron Microscopy). Using mortar cylinders in an accelerated carbonation chamber to obtain results in short lapses, the compressive strength and the carbonation were evaluated. The FTIR analysis results indicate that pH values of 11 and 12 causes a delignification, while at pH 9 and 10, a swelling of the molecule occurs because of the addition of hydroxyl ions, behavior that is confirmed with SEM images. A clear effect of the fiber addition on the performance of concrete was observed as the carbonation front of 35 mm for the sample without fibers was reduced to 2 mm for the sample with 2% fiber addition, resulting in an increase of 5 MPa in compressive strength. These results indicate that in the range of mortar pH, chemical changes occurred over the sugarcane surface that could cause the growth of fibers and could partially seal the porosity in the mortars, thus enhancing its performance.

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