MATERIALS Europe

International Conference on Material Science and Engineering

October 02-04, 2024

ADEIT- University of Valencia, Spain

Abstract book

PRISM

Day 1

Plenary Session

Hysteresis processes in ionic, electronic, and biological devices

Juan Bisquert

Distinguished Research Professor, Instituto de Tecnología Química (UPV-CSIC), Spain

Abstract:

Hysteresis, observed in the current-voltage characteristics of electronic and ionic devices, is a phenomenon in which the shape of the curve is influenced by the speed of measurement. This phenomenon is a result of internal processes that introduce a time delay in the response to external stimuli, causing measurements to depend on past disturbances. Hysteresis and time delay effects find important applications in devices that are explored for resistive switching and neuromorphic computation, such as halide perovskite and organic memristors and transistors for synapses and neurons.

Here we show a classification of various manifestations of hysteresis by identifying common elements. Our approach involves examining hysteresis from multiple perspectives, employing simplified models that capture fundamental response patterns. We investigate system behavior using techniques like linear sweep voltammetry, impedance spectroscopy, and the analysis of transient currents resulting from small voltage steps. Our analysis uncovers two primary types of hysteresis, characterized by how current responds to rapid sweep rates: capacitive hysteresis and inductive hysteresis. These terms correspond to the dominant component in the equivalent circuit, which governs the transient time response. We present the analysis of different materials and devices: halide perovskite memristors, fluidic nanochannels, and organic transistors. We show a classification of the switching response that explains synoptical potentiation and depression, for the realization of neuromorphic circuits. We also explore the formation of artificial spiking neurons based on the previous properties.

Biography:

Juan Bisquert is a Distinguished Research Professor at Instituto de Tecnología Química (Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas). He is Executive Editor for Europe of the Journal of Physical Chemistry Letters. He has been distinguished in the list of Highly Cited Researchers from 2014 to 2023. The research activity of Juan Bisquert has been focused on the application of measurement techniques and physical modeling in several areas of energy device materials, using organic and hybrid semiconductors as halide perovskite solar cells. Currently, the main research topic aims to create miniature devices that operate as neurons and synapses for bio-inspired neuromorphic computation related to data sensing and image processing. The work on this topic combines harnessing hysteresis and memory properties of ionic-electronic conducting devices as memristors and transistors towards computational networks.

Narrow Bandgap Organic Acceptor Materials for Organic Solar Cells

Yongfang Li[1,2]*

[1]*Institute of Chemistry, ICCAS, Beijing 100190, China;*

Abstract

Organic solar cells (OSCs) have attracted great attention in recent years, because of their advantages of simple device structure, light weight and capability to be fabricated into flexible and semitransparent devices. The key photovoltaic materials of OSCs are conjugated polymer donors and *n*-type organic semiconductor (*n*-OS) acceptors. Recently, the low bandgap *n*-OS small molecule acceptors (SMAs) have promoted the research progress of the OSCs significantly.

Here I will report our recent research progress on the narrow bandgap organic acceptor photovoltaic materials, including new narrow bandgap *n*-OS SMAs, polymerized SMAs and the giant molecule acceptors (GMAs) based on the narrow bandgap SMAs, as well as the low-cost polymer donors matching with the narrow bandgap acceptors. In addition, I will talk about our recent results on the perovskite/organic tandem solar cells based on the wide bandgap perovskite solar cell as front cell and narrow bandgap organic solar cell as rear cell.

Biography:

Yongfang Li is a professor at the Institute of Chemistry, Chinese Academy of Sciences (ICCAS) and at Soochow University. He received his Ph. D. degree from the Department of Chemistry, Fudan University in 1986, then did his postdoctoral research at ICCAS from 1986 to 1988. He became a staff in 1988 and was promoted to professor in 1993 in ICCAS. He was elected as a member of the Chinese Academy of Sciences in 2013. He ever did his visiting research at the Institute for Molecular Science, Okazaki, Japan from 1988 to 1991 and at the University of California at Santa Barbara, USA, from 1997 to 1998. His present research field is photovoltaic materials and devices for organic solar cells and perovskite solar cells. He has published more than 900 research papers and the published papers have been cited by others more than 83,000 times with an H-index of 144**.**

Impedance Matching Schemes and Designed Wave Absorption Spectrum

Ping Sheng

Professor Emeritus, HKUST, and Associate at Cambridge University, UK

Abstract

Impedance matching is a pre-condition for a good wave absorber. In this talk I present two impedance-matching schemes, both involving the use of metamaterials, for (a) underwater acoustics, and (b) microwaves. In (a), the combination of the causality constraint and the use of segmented structures is shown to lead to a solid absorber that can impedance-match with water, which sets the stage for resonator integration that can lead to either tunable or near-total underwater acoustic absorption[1]. In (b), a new scheme for impedance matching with the vacuum is presented which involves the use of small metallic rings and their interaction with the image current to produce multiple magnetic resonances. Adding series resistances to the ring flattens the resonances' spectra that leads to impedance matching over a broad frequency spectrum, thereby leading to broadband microwave absorption. The additional use of stacked hierarchical structure further broadens the near-total absorption spectrum, extending from 3 to 40 GHz[2].

Biography:

Ping Sheng is a senior member of the Institute for Advanced Study and Professor Emeritus at HKUST. Since October 2023 he is also an Associate of Clare Hall College in Cambridge University. Prof. Sheng obtained his BSc in Physics from the California Institute of Technology, and PhD in Physics from Princeton University in 1971. After a stay at the Institute for Advanced Study, Princeton, Ping joined RCA David Sarnoff Research Center in 1973. In 1979 he joined the Exxon Corporate Research Lab, where he served as the head of the theory group during 1982-86. In 1994 Ping joined HKUST as a professor of physics and served as the head of the physics department from 1999 to 2008.

Prof. Sheng is a Fellow of the American Physical Society and a Member of the Asia Pacific Academy of Materials. He served as the Executive Editor of Solid State Communications, a Division Associate Editor of Physical Review Letters, and a member of the editorial board of the New Journal of Physics. He was awarded the Brillouin Medal by the International Phononics Society in 2013, the Rolf Landauer Medal by the ETOPIM Society in 2018, and the Bloch Prize in 2021. Prof. Sheng was elected a member of the Hong Kong Academy of Sciences in 2019.

DAY – 2
Session: Novel Materials for Energy and Biomedical Applications
PLENARY TALK

Design and Synthesis of Nanomaterials for Biomedical and Energy Applications (Online)

Jackie Y. Ying
King Faisal Specialist Hospital & Research Centre
Riyadh, Saudi Arabia

Abstract:

Nanostructured materials can be designed with sophisticated features to fulfill the complex requirements of advanced material applications. Our laboratory has developed organic and inorganic nanoparticles and nanocomposites for advanced drug delivery, antimicrobial, stem cell culture, and tissue engineering applications. In addition, we have nanofabricated microfluidic systems for drug screening, *in vitro* toxicology, and diagnostic applications. The nanosystems allow for the rapid and automated processing of drug candidates and clinical samples in tiny volumes, greatly facilitating drug testing, genotyping assays, infectious disease detection, point-of-care monitoring, as well as cancer diagnosis and prognosis.

We have also synthesized metallic, metal oxide, and semiconducting nanoclusters, nanocrystals, and nanosheets of controlled dimensions and morphology. The nano-sized building blocks are used to create multifunctional systems with excellent dispersion and unique properties. Nanoporous materials of a variety of metal oxide and organic backbone have also been created with high surface areas and well-defined porosities. These nanostructured materials are successfully tailored toward energy and sustainability applications

Biography:

Prof. Jackie Y. Ying is the Chair of the Bioengineering and Nanomedicine Department at King Faisal Specialist Hospital & Research Centre. She is internationally renowned for her pioneering research in materials chemistry, with significant contributions to the development of advanced nanostructured materials for catalysis and energy applications. Her innovations include the creation of nanoporous materials, metallic nanoclusters, and nanosystems for drug delivery. Notably, she has developed a groundbreaking insulin delivery system for diabetic patients.
A distinguished leader in her field, Prof. Ying has been honored with numerous prestigious awards, including the American Chemical Society Award in Solid-State Chemistry and the Mustafa Prize. She is also a member of several eminent academies, such as the U.S. National Academy of Engineering and the German National Academy of Sciences.

Keynote Talk

Structural Optimization of Small Molecule Acceptors and Giant Molecule Acceptors and Their Applications in Organic Solar Cells

Xiaojun Li*, Yongfang Li

ICCAS, Beijing, China

Abstract

Organic solar cells (OSCs) have attracted extensive attention in recent years. Our research interests are focused on the design and synthesis of *n*-type organic semiconductor materials and their application in organic photovoltaic devices.

For the small molecular acceptors (SMAs), we revealed the internal reasons for molecular packing and device morphology differences caused by the steric hindrance of alkyl chains and proved that the regulation of the length of alkyl chains is also an important method for modulating molecular packing. In addition, we found the chlorine substitution position of the terminal groups has a regular and significant influence on the molecular packing and photovoltaic performance of the SMAs. These results highlight the importance of the investigation of intermolecular interactions, packing, and the arrangement of the SMAs in the solid state, which may provide direct insights for exploring the relationship between the molecular structure and properties of the photovoltaic materials.

To improve the stability of OSCs and solve the problem of polymer acceptors batch differences, giant molecule acceptors (GMAs) with clear molecular structure and low diffusion coefficients were synthesized. We systematically investigate the influence of the number of SMA subunits in GMAs on the physicochemical, photovoltaic properties and device stability of the GMAs. Furthermore, we applied GMAs to non-halogenated solvent processing and obtained significantly higher efficiency than that of SMAs, which provides a reference for the synthesis of acceptor materials with high efficiency, stability, and green solvent processing.

Biography:

Dr. Xiaojun Li received his Ph.D. degree at the Institute of Chemistry, Chinese Academy of Sciences (ICCAS) in 2019 under the supervision of Prof. Yongfang Li. Then, he pursued his postdoctoral fellowship in Chemistry at the Hong Kong University of Science and Technology (HKUST) under the supervision of Prof. He Yan. He joined the CAS Key Laboratory of Organic Solids, ICCAS as an associate professor in 2021. His research focuses on the design and synthesis of *n*-type organic semiconductor photovoltaic materials and their application in organic solar cells.

Nanostructured optical materials for energy and biosensing applications

Alicia de Andrés

ICMM-CSIC, Spain

Abstract

Reducing the dimensionality of materials provides unique properties that have an enormous impact on a wide variety of applications and has opened new avenues inaccessible to 3D systems. Here a few examples will be presented on how proper nanostructuring of materials confer the resulting system's optical properties fully relevant for energy and sensing applications: The adequate morphology of lead-halide perovskite films and the introduction of graphene are crucial ingredients in the stability and efficiency of solar cells and LEDs. Laser pyrolysis-induced transformation of polymer films yields cost-effective graphic material ideal for flexible electronics and energy storage devices. Structural continuity and optimal porosity of graphene layers are determinants for obtaining laser-induced graphene-based micro-supercapacitors with high capacitance as well as high energy and power densities. The fabrication of a well-designed optical cavity in GaO3:Cr nanowires enables a luminescent and interferometric nanothermometer with excellent temperature range and precision. Finally, 2D-MoS2 can be obtained from nanoflakes to continuous films which triggers an efficient photoluminescence. The variation of this emission when modified with a thiolates DNA probe complementary to the target biomarker can be used as a specific probe to detect the breast cancer biomarker miRNA21c.

Biography:

Alicia de Andrés received her PhD in Physics from the UAM in 1987. She is head of the Heterostructures for Optics and Optoelectronics group and the Optical Spectroscopies Laboratory at the Institute of Material Sciences in Madrid (ICMM-CSIC). Over the last 25 years, she has been researching materials with applications in spintronics and optoelectronics. More recently she has focused on the design, production, and study of 2D materials (graphene and transition metal dichalcogenides) and their symbiosis with nanoparticles for the amplification of optical signals and the development of sensors applicable in different fields such as the detection of biomolecules. In addition, she studies nanomaterials and metal-organic perovskites for light emission, photovoltaic cells, and LEDs. She is the author of more than 190 scientific articles in international WoS journals.

Development of graphene-reinforced magnesium metal matrix composites for biodegradable bone implants

Yuncang Li* and Cuie Wen

RMIT University, Australia

Abstract

There are still several challenges for magnesium (Mg) alloys used as bone implants such as the insufficient mechanical strength and ductility and its rapid degradation in the physiological environment before adequate bone healing. Nano-sized reinforcements have the potential to enhance the mechanical properties of metal matrices. In this study, powder-metallurgy (PM) fabrication routes were used to fabricated new Mg metal matrix composites reinforced with graphene nanoplatelets (GNPs) for biomedical applications. GNPs (0.1, 0.2, 0.3 wt.%) with variable layer thicknesses and sizes were dispersed into Mg powder using high-energy ball-milling processes. The microstructure of the fabricated composites was characterized using transmission electron microscopy, scanning electron microscopy, energy dispersive X-ray spectroscopy, optical microscopy, X-ray diffraction, and Raman spectroscopy. The mechanical properties were evaluated by compression tests. The corrosion resistance was investigated by electrochemical tests and hydrogen evolution measurements. The cytotoxicity was assessed using osteoblast-like cells. The results indicate that GNPs are excellent candidates as reinforcements in Mg matrices for the manufacture of biodegradable Mg implants. GNP addition improved the mechanical properties of Mg via synergetic strengthening modes including grain-refinement strengthening, thermal-mismatch strengthening, dispersion strengthening, and load-transfer strengthening. Moreover, retaining the structural integrity of dispersed GNPs improved the ductility, compressive strength, and corrosion resistance of the Mg–GNP composites. Cytotoxicity assessments did not reveal any significant adverse effects on biocompatibility with the addition of GNPs to Mg matrices. Mg–xGNPs with $x < 0.3$ wt.% may constitute promising biodegradable implant materials for load-bearing applications.

Biography:

Dr Li obtained his PhD in Materials Science Engineering from Deakin University in 2004. He was awarded an Australian Research Council Future Fellowship and won a number of national competitive grants including ARC and Australian National Health and Medical Research Council projects. His research focuses on developing metallic biomaterials for medical applications. He has expertise in microstructure-mechanical property relationships, corrosion, and biocompatibility, surface modification, nanostructured metals and alloys, and metal foams. His research has led to over 280 peer-reviewed original publications, with an H index of 62 and over 12126 citations

Regenerative Materials for a Sustainable Circular Economy

Anke Weidenkaff*, Marc Widenmeyer, Wenjie Xie and Guoxing Chen

University of Darmstadt, Germany

Abstract

The transformation to a future circular economy based on sustainable energy sources such as solar, wind, and geothermal will require huge amounts of new materials. The development and production of novel non-critical materials for catalytic, magnetic, photonic, and thermal converters has to be based on a sustainable and fair use of our resources.

The development of recyclable materials for e.g. renewable green fuel production, storage, transport, and utilization requires large-scale production from secondary raw materials. Future resilient energy systems have to be based on environmental aspects as well as on performance criteria defined by a holistic life cycle assessment. Such goals can be achieved by developing regenerative or self-repairing materials with perovskite structures.

Biography:

Anke Weidenkaff is a W3 professor for Sustainable Materials Science at the Technical University of Darmstadt. Her principal areas of research and expertise are *materials science and resource strategies*, including the development, synthesis, and characterization of sustainable materials for energy conversion and storage. Her current work focuses on regenerative circular materials and the development of next-generation green process technologies for fast and efficiently closed material cycles. Anke Weidenkaff is a member of the German National Academy of Sciences Leopoldina and the National Academy of Science and Engineering acatech.

Excitonic and Electro-Optical Properties of 2D Tin Iodide Perovskites

Juan Martinez Pastor

Universidad de Valencia, Spain

Abstract:

Nowadays, lead halide perovskites have demonstrated great potential for photovoltaic devices (efficiencies over 26 %), light-emitting diodes, photodiodes, and photonic devices. However, the use of lead can reduce the impact of these semiconductors in the production and future commercialization of solar panels and other devices based on them. For this reason, an increasing activity is being developed in tin(II) halide perovskites, for which solar cells with promising efficiencies of over 15 % have been reached recently. In spite of these achievements, further efforts are needed to improve their stability in the air, even after processing under inert conditions. A possible route for such improvement is the use of low-dimensional Sn(II) halide perovskites (Ruddlesden-Popper phases) by introducing certain long organic cations (containing ammonium, amine, etc.). In the present work, we have concentrated on the In the present work, 2D tin(II) halide perovskite 2-thiopheneethylammonium tin(II) iodide, TEA_2SnI_4, has been synthesized in DMF (toxic) and DMSO (non-toxic) solutions and different additives for studying the optical and optoelectronic properties of the resulting films prepared by the scalable inkjet printing technique. Particularly, the combined action of SnF_2 and $NaBH_4$ reducing agents increases the photostability of the resulting films. Room- and low-temperature excitonic photoluminescence (PL), charge carrier recombination dynamics, and micro-PL were used to explain the two excitonic emission bands observed for this 2D semiconductor in the form of polycrystalline thin films, which were associated with the volume and edges of perovskite grains (nanoplatelet-like) composing the films. The study has been also extended to films produced by using SnF_2 and nickel acetate as grain boundaries and TEAI or PMMA as surface passivation, respectively. Photoconductivity measurements were also carried out in encapsulated (inkjet-printed) and unencapsulated (spin-coated) TEA_2SnI_4 films deposited onto ITO-interdigitated electrodes with responsivities in the range of 1-20 A/W at 10 V of bias voltage for the first case and 0.1-10 A/W at 1 V of bias voltage for the second case.

Biography:

Juan P. Martínez-Pastor is PhD in Physics, Full Professor at the University of Valencia, and Director of the Institute of Materials Science (ICMUV). Along his career, he has launched several research labs at ICMUV, supervised 20 PhDs, and published 318 research works (250 papers in JCR journals), six monographs, and one edited book. He has recognized experience & expertise in semiconductor physics (1986-), optical properties and exciton recombination dynamics of low-dimensional semiconductors (1990-), single quantum dot spectroscopy & single photon emission (2004-), optical sensors based on colloidal metal nanoparticles and quantum dots (2007-), active photonic waveguide structures (2010-), photodetectors based on quantum dots and perovskites (2012-), 2D-semiconductors (2013-) and metal halide perovskites (optical properties, recombination dynamics and applications in photonics) since 2014. He has led more than 30 research projects at regional, national, and European levels.

Enhanced Functional Properties of the Multilayered Thin-Film Contacts Based on Cu by Low-Energy Ion Irradiation (Online)

Ivan Kruhlov[1]*, Andrii Orlov, Sergii Konorev, Sergii Sydorenko, Sergey Prikhodko, Svitlana Voloshko

Abstract

Due to their high electrical and thermal conductivity and good electromigration resistance, Cu-based nanoscale thin films are among the most promising materials used in micro and nanoelectronics. However, the problems of enhancing the thermal stability, adhesion strength, corrosion resistance, and functionality of Cu-based contacts are still to be addressed.

In the present study, we applied low-energy (< 2 keV) Ar^+ ion irradiation and complex ion & thermal processing to the multilayered thin films consisting of Ni, Cu, Cr, V layers (each of 25-nm-thick) magnetron sputtered onto Si(100) single-crystal substrate. It was found that the positive effect of complex processing consists in (a) the inhibition of both the external and internal diffusion processes, (b) decreased content of oxygen and carbon impurities in the conductive Cu layer, (c) reduction of oxide sublayers at the internal interfaces, and (d) stabilization of the nanocrystalline structure by inhibiting the recrystallization. To describe the revealed ion-stimulated phenomenon at the interfaces of the studied thin films, model representations are proposed based on the "long-range effect" of low-energy Ar ions. It is also taken into account that due to the increased defectivity of the structure of thin-film materials, the projective ion range in thin films can substantially exceed the values calculated according to Sigmund's theory for bulk materials. In turn, these ion-stipulated features are governing the enhancement of functional properties such as thermal stability, adhesion strength, wear resistance, corrosion resistance, and thus the efficiency of Cu-based nanoscale thin-film materials for micro- and nanoelectronics, photovoltaics, an intelligence-based network of sensors, etc.

Biography:

Ivan Kruhlov was born on June 25th, 1993, in Ukraine. He obtained his Master's degree in Materials Science in 2016, and then his PhD degree in Materials Science in 2023 at Igor Sikorsky Kyiv Polytechnic Institute (Ukraine). In 2016-2019, he was a visiting student-intern in RIKEN SPring-8 synchrotron facility, Japan. His scientific interests lie in the area of nanoscale materials science, thin films, ion irradiation, diffusion, and synchrotron radiation. Currently working in the position of Senior Lecturer and Senior Researcher at the Department of Materials Science & Heat Treatment of Igor Sikorsky Kyiv Polytechnic Institute, Ukraine.

Session: Advanced Functional Materials and Characterization

INVITED TALK

Titanium-Based Laminates Made Using Blended Elemental Powder Metallurgy: Microstructure and Mechanical Behavior (Online)

S.V. Prikhodko

University of California, Department of Materials Science and Engineering, Los Angeles, USA

Abstract

One of the biggest problems for engineering structural materials is that the properties of strength and toughness are mutually exclusive and to date, a meaningful increase of these characteristics in titanium is a big challenge. An approach that uses layered structures can circumvent this problem by using layers of different materials: those with high ductility and high toughness. Titanium-based laminates combining hard metal matrix composites (MMC) and ductile alloy layers are promising materials due to an improved set of mechanical and service characteristics. In the present study, the two and three-layered structures that combine MMC on the base of titanium alloy Ti-6Al-4V (Ti-64) reinforced with 5 to 40 % (vol.) of TiC or TiB particles and the layer made of the alloy Ti-64 were manufactured using press-and-sinter blended elemental powder metallurgy. The effect of processing parameters and the amount of reinforcing phase on the microstructure and mechanical behavior of these materials was analyzed. In addition, hot plastic deformation and hot isostatic pressing of laminates have been used to investigate the potential to improve their microstructure mechanical characteristics. It has been demonstrated that the structures made according to optimized processing parameters exhibit excellent protective performance in ballistic tests. Prospects for improving the structure and methods of making titanium-based laminates are discussed.

BIOGRAPHY:

Sergey Prikhodko, PhD. Director of Materials Structure Characterization Laboratory and Associate Adjunct Professor at the Department of Materials Science and Engineering, University of California Los Angeles. https://cnsi.ucla.edu/materials-structure-characterization-laboratory-mscl/

Area of my scientific expertise lies in the structure characterization of materials using advanced microscopies and spectroscopies including light optical, scanning electron microscopy (SEM), transmission electron microscopy (TEM), high resolution (HR) TEM, focused ion beam (FIB), dual-beam FIB-SEM, scanning transmission (ST) EM, energy dispersive spectroscopy (EDS), x-ray diffraction (XRD), x-ray microscopy, etc. Co-author of more than 100 peer-reviewed publications and more than 70 conference talks. Current research work is focused on the properties of titanium alloys, titanium-based composite, and laminate structures.

Surface engineering of perovskite nanocrystals: sensitization and photocatalytic applications

Raquel E. Galian*

Institute of Molecular Science, University of Valencia

Abstract

The preparation of novel nanohybrids incorporating metal halide perovskite nanocrystals (MHP NCs) has attracted growing interest due to their promising applications in photodynamic therapy, photocatalysis, and photon sensitization. The marriage of MHP NCs with organic dyes offers an effective strategy for creating nanohybrids suited for visible-light harvesting.

This study explores the potential of $CsPbBr_3$ perovskite NCs to transfer energy/charges to surface-attached (4-carboxyphenyl) borondipyrromethene (BODIPY) dyes. A comprehensive set of spectroscopic techniques, including steady-state and time-resolved fluorescence, femtosecond transient absorption spectroscopy, spectroelectrochemistry, and quantum chemical theoretical calculations, were used to investigate the intricate dynamics of excited states within these nanohybrids. The role of iodine substitution in the BODIPY core (I2-BDP) in mediating these energy/charge transfer processes between the MHP NCs and the dyes will be discussed. Additionally, the dual role of the MHP@I2-BDP nanohybrid as a sensitizer of the triplet excited state of I2-BODIPY and serving as an energy transfer photocatalyst for the oxidation of α-terpinene to ascaridole through singlet oxygen generation was demonstrated.

BIOGRAPHY:

Dr. Raquel E. Galian obtained her Ph. D. in Chemistry Science at the Universidad Nacional de Cordoba, Argentina. She did postdoctoral stays at the Polytechnic University of Valencia, the University of Valencia, and the University of Ottawa. She was awarded a Ramon y Cajal contract at the University of Valencia and obtained a permanent position as a Research Scientist in 2017, at the Institute of Molecular Sciences. Her research lines are the "synthesis and functionalization of photoactive nanocrystals and novel nanoarchitecture based on metal-chalcogenide and inorganic/hybrid lead halide perovskites for photocatalysis, and emissive materials".

Modeling damage development during hot forming of super Cr13 at reduced working temperature

Eduardo Garcia-Gil[1]*, Hamed Aghajani Derazkola, Alberto Murillo-Marrodán

University of Deusto, Spain

Abstract

This paper analyzes the effect of reducing the hot forming temperature of superCr13 stainless steel as a means of saving energy and reducing its carbon footprint. For that purpose, hot tension tests of supercr13 cylindrical samples have been carried out at different temperatures (900ºC, 1000ºC, and 110ºC), and rates (0.01 $_{s-1}$,0.1^{s-1}, 1^{s-}1, 10^{s-1}). Results have been used for developing a rheological material behavior model of the material, Hansel-Spittel, and to obtain the critical values of the Latham & Cockcroft damage model. The analysis of these coefficients shows a clear transition in the material behavior between 1000ºC and 900ºC, especially at high strain rates (1^{-1}, 10s^{-1}). At high temperatures and high strain rates, critical damage values are the highest and decrease abruptly at 900ºC, from 0.47 to 0.13 in the case of 10s^{-1}. This behavior is also observed in the resistance of the material; however, the effect of the strain rate is not that relevant. Finally, these models have been applied to the simulation of a hot-forming process to illustrate the validity of the findings. Reducing the forming temperature of this material is an interesting alternative for reducing the environmental impact of the process, however, the limitations arising at 900ºC are to be considered.

Biography:

Eduardo García-Gil is PhD in Mechanical Engineering from the University of the Basque Country, UPV/EHU (July 2014) with Cum Laude and International Mention, specializing in manufacturing. Currently is a full professor at the University of Deusto where he combines lecturing with research in the area of hot bulk material forming: material behavior modeling, friction and wear analysis, and friction stir welding are among his main research topics. Eduardo has 21 indexed publications, 15 of which are Q1. He has wide research experience in research projects from both competitive calls and private funding, being principal investigator in some of them.

Synthesis and characterization of Fe-based magnets for energy applications

Lorenzo-Feijoo, J. P. Andres, N. Coton, J. Ramirez-Castellanos, R. Ranchal1*

Universidad Complutense de Madrid, Spain.

Magnetic ferrites based on iron oxides have been widely studied for decades due to their technological applications, ranging from permanent magnets to microwave absorbers, electromagnetic shielding, and magnetic memory media [1-2]. In this talk, we will focus on Fe-based hexagonal ferrites, which are cost-effective materials for producing sustainable and chemically stable high-coercivity magnets [2-3] for non-demanding applications. Iron-based hexagonal ferrites are among the most widely manufactured magnetic materials, with M-type Sr-based hexaferrite (SrM) being the most used among them [2]. Here, we present our results on Fe-based SrM and BaM hexaferrite's synthesized by ceramic routes, aiming to optimize procedures for fabricating hexaferrite powders for permanent magnets. We used SrCO3 and Fe2O3 as precursors for SrM, mixing them through a ball-milling process and sintering them at various temperatures (from 800 ºC to 1200 ºC) and dwell times. To synthesize BaM we introduce BaCO3 as a reactive component. We correlated microstructure and magnetic properties to optimize the synthesis route. High-quality materials with no secondary phases were obtained under optimized conditions, which showed HC and $BHmax$ values just below recent records reported for ceramic routes [4].

On the other hand, we are also working on the development of bonded magnets for soft magnetic applications such as transformers. Here, the main goal is the development of Fe-based magnetic alloys with low coercivity and high stability [5]. To do that, the NixFe100-x alloys are explored.

References

[1] E. Gorbachev *et al*., Materials Today 32 (2020) 13.

[2] R. C. Pullar, Progress in Material Science 57 (2012) 1191.

[3] P. Maltoni et al., Journal of Physics D: Applied Physics 54 (2021) 124004.

[4] K. Için *et al.*, Materials Chemistry and Physics 290 (2022) 126513.

[5] T. N. Lamichhane *et al*., Mater. Today Phys. 15 (2020) 100255.

Biography:

She began her career in 2000 at UCM, focusing on magnetic materials, and later worked on GaN-based devices with a European Space Agency grant. After completing her PhD in 2006, she became a Full Professor in 2021. Her research spans magnetization control, surface acoustic waves, and energy-efficient magnetic materials. She has supervised theses, led competitive projects, co-authored over 58 articles, and held leadership roles, including Director of *Revista Española de Física* and Coordinator of Materials Engineering at UCM.

Study of the contact behavior of mandrel oxide tribe-layers in the tube piercing process

Alberto Murillo-Marrodan[1]*, Damien Merese[2], Eduardo García[1], Philippe Moreau[2], Jose Gregorio La Barbera-Sosa[2] and Laurent Dubar[2]

University of Deusto, Spain.

Abstract

This study investigates the tribological behavior of the oxide layer that forms on the mandrel during rotary piercing in tube manufacturing. A series of hot upsetting sliding tests were performed to evaluate the oxide layer on hot-working steel under varying contact conditions. Optical microscopy, profilometry, and X-ray diffraction (XRD) were utilized to identify both the contact types and the oxides produced. The findings reveal that abrasive sliding contact occurs between the mandrel and tube materials, with oxide transfer from the tube to the mandrel observed in all test scenarios. Additionally, the oxide layer was shown to reduce the coefficient of friction (COF), confirming its role as a lubricant. The COF was found to decrease with increasing contact pressure and relative velocity. Specifically, as the contact pressure rose from 165 to 200 MPa and the relative velocity increased from 200 to 450 mm/s, the COF dropped from 0.42 to 0.18.

Biography:

Dr. Alberto Murillo is an Industrial Engineer and holds a PhD from the University of Deusto. He is currently Associate Professor at the University of Deusto, where he gives lectures in the area of materials and manufacturing. He has focused his research on the simulation of manufacturing processes using FEM tools, as well as the numerical and experimental characterization of the behavior of metallic alloys at high temperatures, including evaluating contact conditions and their tribological behavior. After completing his doctoral thesis, his field of interest expanded to include friction-stir welding processes, semi-solid forming, and near-solidus forming (NSF). He is currently investigating the potential to extend NSF technology to solid-state recycling and material valorization. He has authored several peer-reviewed publications, book chapters, and presentations at international conferences. He has also participated in several research projects, including european, 4 competitive research projects at the regional level.

GAS-PHASE SYNTHESIS OF NANOPARTICLES: AN ALTERNATIVE PHYSICAL ECO-FRIENDLY ROUTE

Lidia Martínez1 *, Yves Huttel 1

Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC, Spain.

Abstract

Nanoparticles are widely used for many different applications like catalysis, nanomedicine, optics, sensing, etc. Despite the great advances in the field, there is a need for high-precision fabrication methods that can represent an alternative route for some applications. In this sense, the gas phase synthesis of nanoparticles generates a growing interest motivated by different factors like the capacity to fabricate nanoparticles out-of-thermodynamic equilibrium, precise control of the nanoparticle size and size distribution (especially in nanoparticles smaller than 5 nm) or the absence of solvents that enable greener approaches for nanoparticle production [1,2].

In this talk, we will present the last advances of the inert gas condensation method based on magnetron sputtering called sputter gas aggregation source. We will see some examples of the application of these nanoparticles [3] and some of the challenges for their application. In addition, we will present some developments to produce in a more precise way nanoparticles with controllable and tunable size, composition, and structure [4,5].

1. P. Grammatikopoulos at al., PCCP, 25 (2023) 897.

2. O. Kylián et al., J. Vac. Sci. Technol. A, 21 (2023) 020802.

3. F. Fresno et al., Adv. Sustainable Syst. 5 (2021) 2100071.

4. L. Martínez et al., Langmuir, 28 (2012) 11241.

5. D. Llamosa P et al., Nanoscale, 6 (2014) 13483.

Biography:

Tenured Scientist at the Materials Science Institute of Madrid, from the Spanish National Research Council. Her research is mostly focused on the study of nanoparticles, both their manufacture using gas aggregation sources and their characterization using various techniques such as X-ray photoemission spectroscopy (XPS) or atomic force microscopy (AFM). She has made various technological developments to improve the technique of manufacturing nanoparticles using gas aggregation sources. In addition to fundamental studies on the fabrication technique, she also studies the application of nanoparticles in various fields such as nanomedicine, energy, catalysis, and sensor fabrication. She is the author of more than 70 scientific articles and 6 book chapters. She is a co-inventor of 5 patents, three of which are licensed and in exploitation. She is co-founder of two spin-offs of the CSIC, Next-Tip and Nanostine.

Ultrasonic Hologram for Bi-directional Diffusion by Phase Controlling the Scattering Coefficients

V. Romero-García[1*], E. Ballestero[2], J. Rodríguez-Sendra[3], J.-P. Groby[2] and N. Jiménez[3]

Universitat Politècnica de València, València, Spain.

Abstract

In this work, we present a bi-directional asymmetric ultrasonic hologram that can simultaneously control both the reflected and transmitted wave fields. To do that we design a surface made of a discrete spatial distribution of monolithic elements with different properties than the surrounding medium. This allows to compression of two identical or different wavefield scattering patterns (for transmission and reflection) into a single monolithic object. We report an ultrasonic hologram based on Quadratic Residue sequences encoded with resonant building blocks behaving as an ideal Lambertian scatterer from both sides, with spatial autocorrelation coefficients of $\delta \approx 0.7$ each one, therefore diffusing waves in both transmission and reflection. Depending on the applications, such holograms could be useful in situations where transmitted and reflected wavefields need to be controlled at the same time, such as a bi-directional diffusing system emitting and receiving equally in and from all directions (equivalent of perfect optical diffusers in optics) or as a bi-directional beam directivity selector. Such holograms could also be used directly in reflection situations to minimize unwanted specular reflections.

The collaboration between the authors of this article was made possible thanks to the Institut d'Acoustique -- Graduate School (IAGS) project (ANR-17-EURE-0014) from the Laboratoire d'Acoustique du l'Université du Mans (LAUM) for the support and mobility. The authors gratefully acknowledge the ANR-RGC METARoom (ANR-18-CE08-0021). Project. N. J. and V.R.-G. acknowledge financial support from Conselleria de Innovación, Universidades, Ciencia y Sociedad Digital de la Generalitat Valenciana through project CIAICO/2022/052 of the Programa para la promoción de la investigación científica, el desarrollo tecnológico y la innovación en la Comunitat Valenciana. V.R.-G. acknowledges the partial support under Grants from MCIN/AEI PID2023-146237NB-I00, PID2020-112759GB-I00.

Biography:

Dr. Romero-García has contributed to the field of Complex Media. Particularly in the topic of wave propagation in metamaterials and correlated disorder systems. He has contributed to the knowledge of control processes of scattering for absorbing and diffusing waves. His results have been published in journals of high impact factor with an output of more than 100 publications (h-index: 38). After more than 10 years as a CNRS researcher, nowadays is an Assistant Professor at UPV in the Applied Mathematics Department. He has been principal investigator of European, National, and Regional projects and supervisor of more than 10 PhDs and 12 PostDocs.

Session: AI and Computational Strategies in Materials Science
Invited Talk

First Principles Formulation of the Local Functionalization over Time in Two-Dimensional Materials

A.L. Alvarez*1 F. Borrás1, S.J. Quesada1, J. Ramiro1, Alicia de Andrés
Universidad Rey Juan Carlos, Spain.

Abstract

Electric field-assisted covalent functionalization of graphene and other two-dimensional (2D) materials provides robustness and positional control, two crucial features when activating biosensor platforms. In particular, local anodic oxidation has been proven on graphene at the nanoscale since 2008. However, it was not until 2019 that it was demonstrated to have massive application potential, scaling up to hundreds of μm^2 in less than one second. [1] These are sizes required by typical commercial biosensors based on field-effect transistors. Thus, a suitable formulation of the oxidation expansion over time is relevant to control and predict the oxidized spot size on the active biosensor regions. For that purpose, the incorporation of oxyanions at the edge of the oxidized zone has been formulated by applying Boltzmann statistics, which includes physical magnitudes such as the energetic barrier and its dependency on radius and applied voltage. As a result, a function t(r) describing inversely the increase of the spot radius (r) along time (t), is provided. The unknown energetic barrier for incorporation of oxyanions, and its dependency on radius, may be determined by fitting the model to the available experimental data. On the other hand, a simple multilayer stack including the relevant components (oxidized and 2D semiconductor layers, substrate, and metallic contacts) is proposed, where 2D materials are considered as thin films. Under this approach, the Poisson equation has been solved self-consistently by finite element calculations, to obtain electrical magnitudes such as electric field throughout the structure, and the potential drop from the wetting layer to the active material near the edge of the oxidized region. This potential decrease aligns with the potential barrier reduction along the spot radius obtained from fitting the experimental curves, confirming the predictive nature of this model either for graphene or alternative 2D Materials. [1] S. J. Quesada et al., Small, 15 (2019), 1902817.

Biography:

A.L. Álvarez is a full Professor of Electronics at Universidad Rey Juan Carlos, with more than 30 years of experience in Solid State Electronics. In the last 10 years, author of 22 publications in JCR (>300 citations between 2014-23, and two covers in high-impact journals: Small, 40 (2019), and J. Phys. Chem Lett., 6, 11 (2020). Co-inventor of 5 patents (3 international extensions), two best business ideas awards, member of the European Organic Electronics Observatory (2010-2013), Spanish Electron Devices Conference Committee since 2008, and IEEE EDS since 2002. Signatory researcher in 24 competitive projects (6 European), and 8 as PI.

Perovskite Nanohybrid Materials for Optoelectronic and Sensing Applications

Pedro Atienzar*, Kevin Mego, Fernando Ramiro-Manzano, Roberto Fenollosa and Isabelle Rodriguez.

Universitat Politècnica de València, Spain.

Abstract

Accurate knowledge of the optical and electrical properties of 2D nanomaterials is crucial for advancing their use in energy and optoelectronic applications. In this context, synthesizing and studying nanohybrids at the single-crystal scale offers a promising method to explore the intrinsic properties of photoactive materials. This approach avoids the effects of grain boundaries and amorphous domains present in polycrystalline films. Here, we present the optical study of different microstructured materials, such as hybrid perovskites, for developing materials with applications in the fields of energy conversion, optoelectronics, and lighting. For instance, the incorporation of SubPc in the interlayer space of 2D–3D perovskites expand the photoresponse in the visible region. Additionally, significant differences between 3D and multidimensional 2D–3D perovskites under biased detection have been determined. The crystals revealed variations not only in photocarrier decay length values but also in the spatial dynamics across the crystal. Single crystals of hybrid perovskite with appropriate geometry and size constitute Fabry–Pérot-type optical microcavities with well-defined resonances. Such resonances appear in the VIS range when performing optical transmittance or photoluminescence measurements. They strongly depend on the crystal thickness and on the optical constants of the material. These parameters are fundamental for their potential applications in photonic devices.

On the other hand, perovskite nanocrystals with different compositions also show important applications in other fields. For example, gas sensors employing graphene decorated with different perovskite configurations were successfully used to detect pollutant gases at ppm levels.

Biography:

Pedro Atienzar obtained his B.Sc, in Chemical Engineering at the UPV (2002) and did his PhD (2007) at the Instituto de Tecnología Química (UPV-CSIC) under the supervision of Prof. Hermenegildo García. Afterwards, he joined the group of Prof. Jenny Nelson in the Department of Physics at Imperial College London, where he worked as a post-doctoral fellow (2007-2009) in the field of photovoltaics devices. In 2009 he joined the Instituto de Tecnología Química (ITQ). His major research interests are the synthesis and processing of new nanomaterials applied in the fields of photonics, optoelectronics, and renewable energy.

Minimising Dross in L-PBF via Physics Informed Reinforcement Learning

Presenter* and Co-author names (Sam Robbins1*, Ilaria Lagalante2,3, Francesco Careri3,4,5, Moataz M. Attallah3, Leonardo Stella1)

University of Birmingham, United Kingdom

Abstract

Laser Powder Bed Fusion (L-PBF) has rapidly become one of the most successful additive manufacturing technologies, enabling the creation of complex, thin, near-net-shaped metal components. However, one of the main challenges remaining is to ensure dimensional accuracy. This is often compromised by the formation of dross on overhanging structures due to over-melting on downskin layers, caused by the lower thermal conductivity of loose powder. Traditionally, optimizing process parameters to address this issue requires extensive experimentation, demanding significant time and resources. However, artificial intelligence (AI) can assist by making optimization faster and more cost-efficient. This study investigates the application of reinforcement learning (RL) in process parameter optimization for the production of complex thin geometries by L-PBF for Al alloy AlSi10Mg, focusing on the dross minimization and improvement of geometrical accuracy. To achieve this, an RL algorithm (the agent) learns through repeated interaction with an environment. The environment consists of a physics-informed analytical framework for the estimation of melt pool dimensions, based on the Eagar-Tsai thermal model, focusing on the first layers of overhanging struts. This framework was embedded into the environment to guide the agent toward optimal process parameter combinations within a discrete state space. The reward function uses a combination of characteristic numbers through a data-driven reward-shaping process. Experimental data on dross formation from various process parameter combinations were utilized to refine the reward function, enabling the agent to discover better parameter settings that minimize dross and improve geometrical accuracy.

Biography:

I am a PhD student in the School of Computer Science at the University of Birmingham, United Kingdom, under the supervision of Dr Leonardo Stella and Dr Mirco Giacobbe. I have been awarded the departmental scholarship for the full duration of the doctorate. I received a BSc in Physics with first class honors from Keele University, United Kingdom, in 2022, the recipient of the Keele Excellence Scholarship. I completed my MSc Data Science degree at the University of Birmingham, United Kingdom, in 2024, the recipient of the Birmingham Masters Scholarship.

Poster Presentations

Enhancing Catalytic O2 Conversion to H2O2 on Anodic Fe doped Tantalum Oxide Surfaces

Izabela Darowska*, Biswaranjan D. Mohapatra, K. Pawlik, Grzegorz D. Sulka,

Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Cracow, Poland.

Abstract

The electrochemical reduction of O_2 to H_2O_2 is an important process due to its applications in green energy technologies and environmentally friendly chemical synthesis [1]. H_2O_2, a valuable oxidizing agent, can be efficiently produced through the oxygen reduction reaction (ORR) in alkaline or neutral media. Recent studies have shown that catalysts such as semiconducting metal oxides e.g. MnO_2, and TiO_2-based materials demonstrate significant activity for H_2O_2 production under these conditions [1]. In this work, we demonstrated anodic Fe-doped tantalum oxide (Fe-TaOx) structures on Vulcan carbon (VC) as a potential material for electrocatalytic conversion of O2 to H2O2 in alkaline conditions. The Fe-doped Ta oxide (Fe-TaOx) structures were synthesized by anodic oxidation of metallic Ta foils at 15 V, 30 minutes in 0.15 M K4[Fe(CN)6] containing electrolyte (the composition of electrolyte: 90 ml H2SO4 + 6 ml HF + 4 ml H2O). The EDX results indicated about 2 atoms.% Fe in the Fe-TaOx structures. This indicates the suitability of the anodization conditions for incorporation of Fe to anodic TaOx structures. The resulting films were characterized using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and X-ray photoelectron microscopy (XPS). The delaminated and thermally (400°C or 800°C) treated Fe-TaOx were dispersed on VC by ultrasonication to make variations in Fe-TaOx loading on VC (20, 30, 50, and 80 wt.%). The effect of thermal treatment and variation in Fe-TaOx loading on the catalytic conversion of O_2 to H_2O_2 were investigated by RRDE and cyclic voltammetry in 0.1 M KOH. The 800°C treated Fe-TaOx sample with 80 wt.% loading (80 wt.% Fe-TaOx -800/VC) showed ~80 % conversion of O_2 to H_2O_2 at a wide range of applied potential (0.6 –

0.2 V vs. RHE), which is higher compared to other weight loadings (20 and 50 wt.%), as well as also higher compared to Fe-TaOx -400/VC and amorphous Fe-TaOx/VC samples. The 80 wt.% Fe-TaOx -800/VC also showed ~ 2.5 electron transfer number per O2 molecule, demonstrating its high catalytic selectivity of 2 electron transfer for H_2O_2 production. Our results indicate that both thermal treatment and weight % of loading can significantly influence the O2 catalytic activity in these samples.

Acknowledgement:

This research is part of project No. 2021/43/P/ST5/02281, co-funded by the National Science Centre and the European Union Framework Programme for Research and Innovation Horizon 2020 under the Marie Sklodowska-Curie grant agreement no. 945339.

References

[1] G. Maduraiveeran , M. Sasidharan and W. Jin , Prog. Mater. Sci., 2019, 106, 100574

[2] G. D. Sulka Introduction to anodization of metals, *Nanostructured Anodic Metal Oxides*, Sulka, G. D.Elsevier, 2020, pp. 1–34

Biography: I am a graduate of this year's Master’s program in Chemistry from the Faculty of Chemistry at Jagiellonian University. I chose to specialize in Sustainable Chemistry because I believe it is a very relevant and forward-looking direction for contemporary chemistry. I conducted my undergraduate and Master’s theses in the Electrochemistry Group at UJ, where I researched catalysts for photoelectrochemical water splitting.