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ABSTRACT BOOK

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ABSTRACTS

Keynote Session

Spectral Selective Solar Harvesting via Transparent Nano Hybrids for Synergistic Photothermal-Thermoelectric-Photovoltaic Energy Generation

Donglu Shi

University of Cincinnati, OH

Abstract:

In solar applications, the PV efficiencies have been limited by nonideal spectral responses; while the high energy photons contribute to thermalization, the IR portion is responsible for PV heating. We have developed transparent photothermal spectral modulator (TPSM) composed of Fe3O4@Cu2-XS and chlorophyllin compounds, both exhibits pronounced absorptions in the UV and IR regions. Novel hybrids between the porphyrin and iron oxide compounds are also developed for photonically wavelength-modulating photons from UV to IR in a solar energy module that can synergistically generate energy via photothermal (PT), thermoelectric (TE), and photovoltaic (PV) devices. The solar energy module is capable of spectrally distributing photon energies to respective PT, TE, and PV under simulated solar light in the following fashion: 1) photothermally generating thermal energy by TPSM to heat up the hot end of TE for generating electricity; 2) TPSM also functions as a wavelength segregator that removes the IR portion of the light, therefore reducing the PV surface heating, and 3) the PT, TE, and PV are structurally architecture in the solar energy module to fully utilize solar spectrum and produce electricity synergistically. The system efficiency of the novel solar energy module has been found to exceed their commercial PV and TE counterparts. The mechanism of spectral modulation through TPSM is identified based on the photonic behaviors of chlorophyllin, Fe3O4@Cu2-XS, and their hybrids.

Biography:

Dr. Donglu Shi is currently the Professor of Materials Science and Engineering at the University of Cincinnati. Dr. Shi's research encompasses a wide range of fields, including nanoscience, energy materials, nano medicine, and condensed matter physics, resulting in more than 300 peer-reviewed journal publications including ones in Nature, Physical Review Letters, Advanced Materials, and ACS Nano. He is currently the Editor-in-Chief of Nano LIFE, Editorial Board of Biomaterials Advances, and Associate Editor of J. of Nanomaterials. He has received 2023 Rieveschl Award for Distinguished Scientific Research, SIGMA XI Research Recognition Award, and Neil Wandmecher Teaching Award. Donglu Shi is a Fellow of ASM International.

Density Functional Theory Optical and Electronic Properties of MoS2-Graphene-Metal Heterointerfaces

Nikolaos Dimakis

University of Texas Rio Grande Valley, TX

Abstract:

We present preliminary results on density functional theory calculated electronic information and optical properties on heterointerfaces formed by molybdenum disulfide monolayers, graphene, and various metals. Adding a second layer of MoS2 changes the MoS2 bandgap from direct in the monolayer to indirect in the bilayer in a similar fashion as the bulk MoS2. The addition of this second layer does not affect the MoS2-metal distance. We found that graphene insertion between the MoS2 and the metal breaks the graphene cones and introduces band gaps in the Fermi energy for the cases where the metal is Pt and Ni. These bandgaps in the Dirac cone region strengthen π→ π transitions, which is evidenced by the out-of-plane components of the frequency-dependent dielectric function imaginary part. Sulfur vacancies introduce fact bands in the MoS2 band structure. For the MoS2/Au, the in-plane component of the dielectric function shows peaks in the sub-eV region, indicating intraband transitions within flat bands at the Fermi energy, whereas the out-of-plane component is minimally affected due to the presence of these vacancies. For MoS2-Metal configurations, electron transfer from metal to MoS2 is observed, causing the MoS2 monolayer to be an n-type semiconductor, whereas graphene becomes electron deficient in MoS2-graphene-metal cases and thus a p-type semiconductor. We also discuss future work on using GW and

BSE approaches to account for e-e and e-h interactions.

Biography:

Dr. Nikolaos (Nicholas) Dimakis is a Full Professor and Department Chair at the University of Texas Rio Grande Valley. He graduated with a Ph.D. in Physics from the Illinois Institute of Technology (IIT) in Chicago. He worked at the IIT collaborative accesses team at the Advanced Photon Source beamline for several years before joining UT Pan-American as an Assistant Professor in 2004. His research is on computational material science applicable to various materials such as platinum-based alloys, heterostructures, and pyrochlores. He has over 55 peer-reviewed publications and participated in externally funded grants of about $8M.

Precipitation Processes in a Ti-15Mo Alloy

Milos Janecek

Charles University, Czech Republic

Abstract:

Metastable beta titanium alloys are perspective candidates for the use in the aircraft industry and medicine due to their excellent strength, relatively low modulus of elasticity and enhanced biocompatibility. Thermomechanical treatments are often used to improve mechanical properties of these alloys due to the precipitation of different phases, namely the α- and ω-phase. Moreover, α-phase precipitation is known to be heterogeneous and preferentially occurs at lattice defects as e.g dislocations, grain boundaries, etc. A Ti15Mo, which is a representative of a simple binary metastable beta Ti alloy, in a beta solution treated condition was subjected to severe plastic deformation by high pressure torsion (HPT) to produce an ultrafine grained (UFG) material. The material both in the initial coarse grained (CG) and UGF conditions was subsequently heat treated to examine the kinetics of precipitation and to obtain a material with optimum mechanical properties. The effect of induced strain and local chemical inhomogeneities on precipitation was examined by in-situ experimental techniques, namely synchrotron X-ray diffraction and electrical resistivity. The research was subsequently complemented by post-mortem detail investigation of the microstructure in both conditions employing scanning and transmission electron microscopy including advanced techniques of transmission Kikuchi diffraction and automated crystallographic orientation mapping, positron annihilation spectroscopy, and X-ray diffraction.

Biography:

Prof. Miloš Janeček studied physics at the Charles University, Prague, Czech Republic and defended his PhD at 1992 at the same University. After a two-year post-doc fellowship at the University of Manitoba in Winnipeg, Canada and another 18-months fellowship at the LTPCM INP Grenoble, France, he worked as a visiting professor at the Clausthal Faculty of Technology, Clausthal, Germany. In 2017 he became a full professor at the Charles University. His research interests include: microstructure investigation; physical properties of materials processed by severe plastic deformation and additive manufacturing; phase transformations in metastable Ti and Zr alloys and HEAs.

Magnon-Phonon-Photon-Plasmon Coupling in 2D Artificial Magneto-Elastic Crystals

Supriyo Bandyopadhyay

Virginia Commonwealth University, VA

Abstract:

A two-dimensional artificial magneto-elastic crystal consists of a periodic array of magnetostrictive nanomagnets (100-300 nm lateral dimensions) deposited on a piezoelectric substrate. A surface acoustic wave (SAW) launched in the substrate acts as a source of phonons which excite spin waves (magnons) in the nanomagnets via magneto-elastic (or magnon-phonon) coupling. These magnons can, in turn, couple with radiative photons and radiate electromagnetic waves in space (tripartite phonon-magnon-photon coupling) 1. We have studied the coupling modalities and the associated features with time-resolved magneto-optical Kerr effect (TR-MOKE) microscopy.

Additional features can be observed in bilayer magnetic dots that have a layer of plasmonic material (e.g., Al) in them. Surface plasmons from the Al hybridize with phonons sourced from the SAW to produce a hybrid acousto-plasmonic excitation that excites spin wave frequency combs in the samples owing to

strong non-linear tripartite coupling between the phonons, plasmons and magnons. We have observed two octaves of spin wave frequency combs (in the GHz regime) with TR-MOKE. There is also evidence of large parametric amplification where energy is transferred from the acousto-plasmonic mode to spin wave modes efficiently2,3. The large coupling efficiency (estimated cooperativity factor much larger than unity) hints at the formation of a new quasi-particle that we call "magnon-plasmon-polariton". We have also observed tripartite magnon-phonon-magnon coupling (coupling between two Kittel type spin wave modes and a magneto-elastic mode of mixed magnon-phonon character) in a two-dimensional artificial magneto-elastic crystal4. Again, the coupling is strong enough to form a new quasi-particle – a "binary magnon-polaron".

Biography:

Supriyo Bandyopadhyay is the Commonwealth Professor of Electrical and Computer Engineering at Virginia Commonwealth University where he directs the Quantum Device Laboratory. Research in the laboratory has been frequently featured in national and international media (newspapers, internet blogs, magazines such as Business Week, journals such as Nature and Nanotechnology, TV networks such as CBS, radio such as NPR, and several internet news portals). Prof. Bandyopadhyay has received many awards and has authored and co-authored over 400 research publications and presented over 150 invited talks and colloquia across six continents. He served as a Jefferson Science Fellow of the US National Academies of Science, Engineering and Medicine during 2020-2021 and was assigned as a Senior Adviser to the US Agency for International Development (USAID) Bureau for Europe and Eurasia, Division of Energy and Infrastructure. Prof. Bandyopadhyay is a Fellow of the Institute of Electrical and Electronics Engineers, the American Physical Society, the Electrochemical Society, the Institute of Physics (UK) and the American Association for the Advancement of Science.

Doping in Diamond and Diamond as an Electronic Material - Diamondtronics

M S Ramachandra Rao

IIT Madras, India

Abstract:

Diamond is a remarkable and versatile material, due to its potential applications in quantum technologies, high-frequency and power electronics, mechanical uses, and thermal management. With an ultra-wide bandgap of ~5.5 eV, diamond facilitates the development of robust power devices such as field-effect transistors and high-voltage diodes. Despite being one of the most resistive materials, diamond can transition to a semiconducting and to superconducting states via boron doping. Boron-doped diamond (BDD) is considered a promising next-generation granular superconductor, particularly useful for quantum-interface devices requiring high surface inductance [1,2]. The exploration of wide bandgap quantum systems hinges on effective doping, which, although feasible in diamond lattices, presents challenges during the CVD growth process. Nitrogen-doped diamond shows potential for quantum computing and magnetometry applications. Its ultra-wide bandgap enhances the efficiency and longevity of RF devices by minimizing power losses, increasing breakdown voltages, and improving heat dissipation. An alternative method, known as 'surface transfer doping,' leverages the negative electron affinity of hydrogen-terminated diamond. Our research group has achieved stable superconductivity in boron-doped diamond, and the implantation of nitrogen and phosphorus has shown improved conductivity [3]. We also focus on growing single-crystalline diamond with reduced defect concentrations. Techniques such as Raman linewidth, photoluminescence spectroscopy, UV-Vis, and FTIR spectroscopies are employed for quantitative defect analysis. Diamond is poised to be the next-generation material for Diamondtronics.

Biography:

Prof. M.S. Ramachandra Rao is a Chair Professor at IIT Madras and a fellow of the Institute of Physics (FInstP), UK. He was an Alexander von Humboldt (AvH) fellow (Germany); JSPS fellow and JST fellow (Japan); visiting faculty at the University of Maryland, College Park from 2002-2004 (USA); visiting faculty in the ERASMUS-MUNDUS master's program (MaMaSELF) since 2005 (France, Germany and Italy) and an adjunct faculty of Shibaura Institute of Technology (SIT) (Japan). He has supervised 30 PhD students, and about 100 undergraduate and postgraduate students; published about 350 research papers in peer-reviewed journals. He has about 25 patents and 5 technology transfers. With a big grant from the government of India, Prof. MSR Rao's group is all geared up for developing equipment and processes to produce and explore diamonds not only as gem crystals but also as the next-generation semiconductor and electronic material for a plethora of applications.

Topographic Scanning Electron Microscopy Revealing the Three-Dimensional Surface Structure

Ouyang Jianyong

National University of Singapore, Singapore

Abstract:

Scanning electron microscopy (SEM) is a very popular technology to analyze the surface morphology of various materials in both academia and industry. Its principle is the detection of secondary electron emission and electron scattering interactions between the electron beam and the sample surface. It requires the deposition of a thin metal film like Au on non-conductive samples to prevent charge accumulation. However, due to the discontinuity of the Au film along the vertical direction of a sample, the SEM images cannot provide information along the vertical direction. Additionally, the gold films have grains of 10–12 nm in diameter, which can limit the resolution of the SEM images.

In this talk, I will present a new technology called topographic SEM that reveals the three- dimensional surface structure of materials. A non-conductive sample is coated with poly(3,4-ethylenedioxythiophene):poly (styrenesulfonate) (PEDOT:PSS, an intrinsically conductive polymer) onto samples instead of metal deposition for SEM. High-quality features along both the horizontal and vertical directions can be observed on the SEM images because PEDOT:PSS can form a continuous film along both directions. Furthermore, due to the featureless morphology of the PEDOT:PSS films, the resolution of SEM images is significantly higher than that with gold deposition. The application of topographical SEM in the characterization of various materials, including patterned semiconductors, nanostructured materials, energy materials, biomaterials, etc is demonstrated.

Surprises from MAPbI3: Beyond its Optoelectronic Properties

Dipankar Das Sarma

Indian Institute of Science, India

Abstract:

The last fifteen years have seen the most spectacular rise of a class of materials centered around the hybrid halide perovskite, MAPbI3. Their optoelectronic properties, primarily photovoltaic, light-emissive, and detection properties have reached superlative performance levels within this exceptionally short period and have taken the world by surprise. The community's preoccupation with such spectacular properties, however, has hindered closer scrutiny of their many other intriguing behaviors; we shall discuss two puzzling properties of MAPbI3 that we discovered recently.1,2 The first example1 deals with the realization that the thermal conductivities of MAPbI3 and related compounds are not only ultra-low but are even considerably lower than the minimum thermal conductivities expected from such materials in the extremely disordered, glassy limit. We probe this issue to understand how the thermal conductivity of a crystalline solid can be lower than its glassy, minimum thermal conductivity limit. In the second example, we show that MAPbI3 has the peculiar ability to code its thermal history in its structural evolution within the hysteretic region of its first-order phase transition; we further show that photoluminescence signal provides a convenient and robust readout method to probe these unique microstates with extreme accuracies.

Oral Presentations

Emerged speakers

Improving Biodegradable Mg-Zn(-Ca) Alloys by PEO Surface Treatment

Peter Minarik

Charles University, Czech Republic

Abstract:

This study investigates the influence of plasma electrolytic oxidation (PEO) preparation time on the degradation resistance of Mg-1Zn (Z1) and Mg-1Zn-0.4Ca (ZX10) alloys, with comparisons to pure Mg and commercial Mg-4Y-3RE-0.4Zr (WE43). PEO layers were formed with varying preparation times (5, 10, and 15 minutes) and analyzed for microstructure, morphology, and corrosion resistance. Results indicate that PEO layers with a 10-minute preparation time exhibit the most homogeneous structure and optimal corrosion resistance. Prolonged PEO preparation times increased pore density, crack formation, and layer thickness, while also promoting layer degradation during extended immersion in 0.9% NaCl corrosive media. The dissolution of phosphates from PEO layers contributes to the formation of a protective corrosion layer, enhancing long-term resistance. These findings demonstrate that low-alloyed, biocompatible Mg-Zn(-Ca) alloys can achieve corrosion resistance comparable to high-performance WE43 alloys through appropriate surface treatment.

Biography:

Peter Minarik is an associate professor at Charles University, Department of Physics of Materials, where he also defended his PhD. in 2014. He co-authored over 190 research papers indexed in the Web of Science database. His major scientific interest is biodegradable metallic materials, but as an expert in scanning electron microscopy, he participates in developing various structural materials.

PCT-Based Smart Heaters from Conductive Polymers

Petr Spatenka

Czech Technical University in Prague, Czech Republic

Abstract:

Conductive composite polymers with PTC effect are promising material for simple and cheap production of smart self-regulating heaters. However, the poor reproducibility after repeated temperature cycles is a limiting factor for their industrial application. To address this problem, we performed number of experiments with samples made by injection molding from commercially available conductive HDPE composite material Sabic 8520. The square-form samples were equipped with sputtered c0pper contacts, and which were connected to a power supply. The time dependence of temperature was studied. To investigate the time stability the heating was repeated on selected samples. A decrease in the current with time was observed resulting in high irreproducibility leading to sample distortion after several cycles. Based on the experimental results combined with theoretical calculation we have found the reason of the current decrease was in a small inhomogeneity in the sample conductivity. Due to positive feedback, this high resistivity area extended across the sample forming a line-like structure parallel to the electrodes which hinders the current flow and thus heating of the sample. Microscopic investigation indicated that agglomeration of the conductive fillers in the line-like structure resulted in breaking the conductive paths. The negative effect can be eliminated by splitting the heating area into several separate sections. Another method for reproducibility enhancement was in formulation composite material where the carbon black was replaced with small carbon fibers.

Biography:

Petr Špatenka received the M.Sc. degree in physics and mathematics and the Ph.D. degree in plasma physics from the Charles University in Prague. He is professor at the Czech Technical University in Prague and Faculty of Agriculture at the University of South Bohemia in České Budějovice. His research interests include functional plastics, composite materials, plasma chemical processes and their application for surface treatment. He is an author or co-author of over 100 peer-reviewed articles, several patents, numerous conference contributions and three book chapters. He is the founder of the Plasma Tech Ltd. and the Surface Treat Inc. companies.

Organic Mixed Ionic-electronic Conductors for Electrochemical Applications

Penghui Ding

Stanford University, CA

Abstract:

Coupling between ions and electrons is important for a host of electrochemical applications underpinning societal needs from batteries to electrolyzers. Organic materials that efficiently support both ionic and electronic transport have received much attention in the past few years as ideal materials for such applications owing to their processability and more recently for their coupled transport properties. Organic mixed ionic-electronic conductors (OMIECs) are soft electrical (semi-)conductors, predominantly polymers, that solvate and transport ions. In addition, the intrinsic elasticity and structural customization of OMIECs make them favorable for diverse electrochemical applications. However, direct use of OMIECs in electrochemistry excluding supercapacitor field is still scarce now. Our group have recently leveraged the decade-long experience in OMIECs research for electrochemical processes, such as electrochemical thermogalvanic cell, oxygen reduction reaction, aqueous organic redox flow battery, and stretchable battery. 1-9 We investigated the effects of electronic and ionic conductivity of OMIECs on those processes and translated the understanding so gained into relevant electrochemical devices.

Biography:

Penghui Ding is a postdoctoral scholar in Prof. Richard N. Zare's group on the physicochemical properties of bubbles and droplets for sustainability at Stanford University, USA. Previously he received PhD in Applied Physics at Linköping University, Sweden with Prof. Reverant Crispin working on organic materials-based electrochemical flow cells for energy applications, such as electrolyzers and flow batteries in 2024. His focus is fundamental understanding and system development of various sustainable technologies, such as (photo)electrochemical devices, redox flow batteries, and microdroplet chemistry.

Flexible Organic Electrochromic Devices Having Multicolored, Low-Voltage-Driven and High Contrast, and Organic Photovoltaic Properties Based on Oligomers and Viologen Derivatives

Ping Liu

South China University of Technology, China

Abstract:

A series of organic conjugated oligomers and viologen derivatives are synthesized, their photovoltaic (OPV), electrochromic (OEC) properties and corresponding flexible electrochromic devices (FOECD) were investigated. The research results of OPV showed that the hydrogen bond interaction between electron donor and electron acceptor, and photovoltaic materials with liquid crystal and crystal properties, can improve the photoelectric conversion efficiency (PCE) of organic photovoltaic devices. The research results of OEC showed that these oligomers and viologen derivatives exhibit reversible color changes upon electrochemical doping and dedoping. The FOECD has high optical contrast is 75.2% at 700 nm. Furthermore, FOECD driven by solar cells demonstrated good stability.

Biography:

Ping Liu is a professor in the School of Materials Science and Engineering and the Institute of Materials Science in South China University of Technology (SCUT). He received his B.S. and M.S. degrees from Sun Yat-sen University in 1986 and 1991, respectively, and his Ph.D. degree in Materials chemistry from Osaka University in Japan in 2000. He joined the Institute of Materials Science, South China University of Technology (SCUT) in 1991, and became a full professor in 2005. His research focuses on organic/polymer functional materials, including organic/polymer optoelectronic materials and devices, organic/polymer flame retardants and flame-retardant material, adhesives for automotive, pressure sensitive adhesives for power batteries, etc.

Recycling of Primary Spent Batteries Solution Through the Precipitation of Zeolitic Imidazolate Frameworks and Revalorization into Anode Materials for Li-ion Batteries

Despoina Andriotou

University of Grenoble Alpes, France

Abstract:

Up to this day, the recycling process in primary batteries involves (hydro) metallurgic processes to produce drip trays, a rather high cost procedure for a low cost material. Herein, we report a closed recycling loop, starting by the selective precipitation of zinc into Zeolitic Imidazolate Frameworks (ZIFs) from a polymetallic aqueous solution, derived from a black mass sample of alkaline (primary) batteries containing metals like Zn, Mn, Ni, Cu, Al, Fe and Co. The synthesis conditions were adapted to meet the industrialization needs (water as solvent and sulfate precursors). With the help of benzimidazole or 2- methylimidazole, ZIF-7-III and ZIF-8 precipitated accordingly, leading to a recovery of more than 99 % of zinc in a one-step and one-pot reaction. Both materials (ZIF-7-III and ZIF-8) were fully characterized and then underwent a thermal treatment under hydrogenated argon atmosphere (2% H2/Ar), forming metallic zinc (Zn0) that was collected with a recovery rate between 85-95% of metallic zinc and could be involved in the making of new alkaline batteries. At the same time, all by-products of the closed loop are investigated to be revalorized in other applications. Notably, we are able to isolate the organic residue of imidazolate-derivatives and form hard carbon and graphite like materials shaped in spherical particles with high taped density up to 2.5 g/cm3.Electrochemically, these carbons show to be good candidates as anode material for rechargeable Li-ion batteries with a specific capacity of 200-300 mAh/g and a great stability in cycling.

Biography:

Dr. Despoina Andriotou, originated from Greece, obtained her PhD in material chemistry in 2023 from the University of Lille. Specialized in porous materials (Metal-Organic Frameworks,zeolites) she possesses a strong background in material synthesis and characterization. During her career, she studied different hybrid porous materials for optical, luminescent, biomedical and nuclear applications. In her latest post in CEA (French Alternative Energies and Atomic Energy Commission), she has the opportunity to focus on green chemistry and assist in the energy transition, through the development of innovative recycling processes for batteries and the revalorization of by-products to valuable materials.

Plastic Instabilities and Microplasticity in FeAlCr-based Complex Concentrated Alloys

Michal Knapek

Charles University, Czech Republic

Abstract:

Complex concentrated alloys (CCAs) typically feature various unique and attractive properties, such as good strength and stability at high temperatures. Due to the concept of high concentration of multiple elements in CCAs, the plastic deformation activity is intricate and still far from fully understood in these materials. In this study, we investigate plastic instabilities and microplasticity in equiatomic FeAlCr-based medium-entropy alloys in compression. Initial studies of deformation mechanisms revealed an unusual, serrated flow observed around 400 °C and a strain rate of 10-4 s-1. Temperature and strain rate were systematically varied to assess their impact on deformation behavior. Compression curves and strain rate jump tests indicate that the jerky plastic flow is attributed to dynamic strain aging manifested as the Portevin-Le Châtelier (PLC) effect. The compression tests are also correlated with the concurrently recorded acoustic emission (AE) data. The AE results provide evidence that considerable (micro)plastic activity occurs already during quasi-elastic loading. Statistical analyses of AE data further suggest that the serrated flow results from sequences of dislocation avalanches with magnitudes following the power-law distribution, thus bearing witness to stochasticity, self-organization, and universality of elementary plastic events.

Biography:

Dr. Michal Knapek received his PhD degree in 2016 at the Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic, where he also obtained the position of Assistant Professor in 2022. He has published more than 60 research papers indexed in the Web of Science database and his current research interests include deformation characteristics of solids, plastic instabilities, micromechanical testing, and in-situ monitoring of deformation dynamics.

Critical Chloride Thresholds and Mechanisms of Corrosion Initiation in Low-Carbon Steel Rebar

Ebenezer Fanijo

Georgia Institute of Technology, GA

Abstract:

Chloride-induced corrosion is the leading cause of reinforced concrete degradation, accounting for 70% to 90% of premature structural failures. Despite the well-documented consequences of corrosion damage (e.g., cracking, spalling, and reduced structural capacity), the initiation and propagation mechanisms of chloride-induced corrosion remain poorly defined. For instance, the critical chloride content (Ccrit) required to initiate corrosion has been inconsistently reported in the literature, with values ranging from 0.04% to 8.34% by cement weight. This study utilizes potentiostatic control and in spectral modulation interferometry (SMI) technique to determine the critical chloride content (Ccrit) required for corrosion initiation on direct low-carbon steel rebar. Chloride threshold values were assessed across a range of concentrations (0 - 5.0% by weight) in simulated pore solutions under flowing conditions. Lower chloride concentrations maintained the passive film, while higher concentrations accelerated corrosion initiation, with current transient's characteristic of pit initiation, passivation, and propagation stages. The quantitative analysis of the height profile data (acquired from SMI) verified the heterogeneity of the corrosion process of these samples susceptible to pitting corrosion and intergranular corrosion behavior. These results underscore the critical role of chloride concentration in the early stages of corrosion and its relationship with reinforced steel degradation. The findings from this study contribute to a more accurate prediction of chloride- induced corrosion initiation and propagation rates and mechanisms, particularly in relation to the micro- and nanostructural behavior of reinforced concrete.

Biography:

Dr. Ebenezer Fanijo is an Assistant Professor in the School of Building Construction at Georgia Tech. His expertise lies in sustainable and resilient buildings and civil infrastructure, with a particular focus on decarbonizing infrastructure through novel low-carbon construction materials and alternative energy sources. His research encompasses cementitious and concrete composites, corrosion monitoring and mitigation, green concrete technology, 3D printing of cementitious materials, structural health monitoring, and advanced sensing technologies. Dr. Fanijo has co-authored over 20 peer-reviewed articles and conference proceedings. In addition to his academic contributions, he is a licensed Professional Engineer with over a decade of experience in the construction industry.

Based on Group III-Nitride Materials High Electron Mobility Transistors for mmWave Applications

Hao Lu

Xidian University, China

Abstract:

AlGaN/GaN-on-SiC high-electron-mobility transistors (HEMTs) have emerged as a focal point in advanced semiconductor research, primarily due to their exceptional power handling capabilities, which surpass those of conventional Si CMOS and III-V compound materials. With the escalating demands of modern communication systems, particularly in high-frequency and high-power applications, there is an urgent need to enhance the performance metrics of power amplifiers (PAs), specifically their output power and linearity. While our prior investigations into AlGaN/GaN HEMTs have yielded notable achievements, including power densities exceeding 33 W/mm in the X-band and 14 W/mm in the Ka-band [1], conventional AlGaN/GaN heterostructures face significant limitations in meeting the stringent requirements of millimeter- wave applications. These limitations stem from pronounced short-channel effects and inherent nonlinearity issues, which degrade device performance at higher frequencies. To overcome these challenges, innovative approaches to epitaxial structure design are essential, offering a pathway to optimize device characteristics and address the critical bottlenecks in millimeter-wave performance. In this presentation, we introduce a novel multiscale vertical scaling-down epitaxial structure design, featuring an AlN/GaN/InGaN architecture, specifically engineered to address key challenges in millimeter-wave (mmWave) applications. This design aims to mitigate the short-channel effect, strengthen quantum well confinement, and improve thermal management. The incorporation of coupling channel engineering demonstrates a significant reduction in dynamic source resistance, leading to enhanced transconductance (gm) and RF linearity. Furthermore, the AlN/GaN/InGaN coupling channels achieve an exceptional

subthreshold slope of less than 60 mV/dec with the underlying hot electron transfer mechanism providing a theoretical foundation for these performance gains.

Biography:

Hao Lu, Ph. D. is a postdoctoral researcher at Xidian University, China. He received the Ph.D. degree in electrical engineering from Xidian University, Xi'an, China in 2022. He has been engaged in the research of GaN-based microwave/millimeter wave electronic devices and key technologies of heterostructure integration for a long time. He has published 38 technical papers in international high-level journals and conferences such as IEEE Electron Devices Letters, IEEE Transactions on Electron Devices, Applied Physics Letters, IEDM, etc., including 15 first-author publications and 22 chinese filed/pending patents. He has made several oral reports at international conferences such as IEDM, IEEE WiPDA, IEEE ICTA, IWN, APWS, CSW etc. In 2021, he won the IEEE WiPDA-Asia Best Presentation Award, AMSE Best Presentation Award, and Xidian Excellent Doctoral Dissertation Funding. Dr. Lu is Member of IEEE, China Institute of Electronics (CIE), and Chinese Physical Society (CPS). His specific research interests include the advanced fabrication, characterization, and integration of wide band-gap semiconductor electronic devices.

Facile Synthesis and Efficient Nickel-based Photothermal Catalyst for Selective Production of CH4 and CO

Guoshu Deng

Southeast University, China

Abstract:

CO2 hydrogenation is not only a significant technical route for carbon emission reduction but also contributes to the production of various value-added chemicals. Nickel (Ni) has been extensively employed in catalytic conversion of CO2 due to its wide accessibility, lower cost and good activity. Herein, the catalysts for CO2 hydrogenation were prepared by loading Ni on mesoporous silica with highly ordered mesoporous structure, which effectively improves the dispersion of metal particles and prevents the sintering at high temperatures. Besides, the addition of La2O3 as promoter in the Ni-based catalyst gives rise to the number of medium basic sites and mitigates the recombination of photogenerated electron-hole pairs, which reinforces the catalytic performance in CO2 hydrogenation. In this study, the introduction of light irradiation at 500 °Clead to the transferring of electrons from SiO2 to Ni2+ and La3+, which is different from that at room temperature with the electrons flow from La3+ to Ni2+. Moreover, the catalyst exhibits the highest Ni0/Ni2+ ratio under photothermal conditions, which results in the considerable CO2 conversion of 70% and CO selectivity of 97%. The satisfying dispersion effect of mesoporous silica and the stable photo-electric conversion ability of La2O3 modified Ni-based catalyst bring about the fulfilling stability in long-term photothermal catalytic reactions. More importantly, CH4 or CO could be selectively obtained with high selectivity (>95%) by adjusting the photothermal catalytic conditions via simple operation. It is envisage that the catalyst and technical method in this study holds great potential in practical industrial production.

Biography:

Guoshu Deng received her master degree from University of Glasgow in 2021, and she is currently a Ph.D. candidate at Southeast University. Her research focuses on integrated CO2 capture and conversion with dual-function materials, with the aim of simultaneously capture CO2 from simulated flue gas (low CO2 concentration) and convert it into value-added chemicals such as methane, which saves great energies and expenses in the process of incurred in CO2 compression and transportation processes of conventional carbon capture, utilization, and storage (CCUS) technology.

Characterization of Photoconductive UV Sensors Using ZnO Single Crystal Substrates and Thin Films

Takami Abe

Iwate University, Japan

Abstract:

Zinc oxide (ZnO) is a direct transition-type wide-bandgap semiconductor with a bandgap energy of 3.37 eV and a large exciton binding energy of 60 meV. Owing to these properties, ZnO is considered a prom-

ising material for ultraviolet (UV) optoelectronic devices such as UV light-emitting diodes (LEDs) and UV photodetectors. When used as a UV sensor, ZnO can be implemented in two major types: photoconductive and Schottky-based sensors. In this study, we investigated a photoconductive-type UV sensor, which offers high photoconductive gain and ease of fabrication, and evaluated its characteristics. For the experimental investigation, ZnO single-crystal C-plane substrates with Zn-face and O-face orientations were used. The results showed that rapid thermal annealing (RTA) at 600°C for 3 seconds in an oxygen atmosphere significantly enhanced the photoconductive response of the Zn-face substrate. This improvement is attributed to the reduction of oxygen vacancies and the optimization of carrier transport properties. Furthermore, ZnO thin films were deposited on sapphire A-plane substrates using the plasma-assisted reactive evaporation (PARE) method to fabricate photoconductive UV sensors. The structural and optical properties of the deposited thin films were evaluated using X-ray diffraction (XRD) and photoluminescence (PL) spectroscopy. Additionally, the photoconductive response under UV illumination was measured, demonstrating the potential of ZnO thin films for UV sensor applications. In this presentation, we will discuss the effects of thermal treatment on ZnO single-crystal substrates, the fabrication process of ZnO thin-film-based UV sensors, and their photoconductive properties.

Biography:

I, Takami Abe, received a Ph.D. in Engineering from Iwate University. I am currently an Assistant Professor at the Faculty of Science and Engineering, Iwate University. My expertise is in electrical and electronic engineering and crystallography. My research focuses on ZnO-based UV LEDs, UV sensors, radiation detection, and hydrothermal synthesis of ZnO single crystals.

Liquid Metal Jetting for Electrode Fabrication on Glass Substrates

Manoj Meda

Corning Inc., NY

Abstract:

This study investigates the use of liquid metal jetting (LMJ) for the creation of highly conductive electrodes on glass substrates, specifically wrap-around electrodes in advanced display applications. Using Corning's display glass and aluminum alloy 4008, we achieved printed features with widths of 250 μm and thicknesses of 200 μm. The LMJ method, which utilizes a magnetohydrodynamic ejection system to deposit molten metal droplets, offers numerous advantages over traditional printing techniques, including bulk conductivity, no need for post- processing, and cost-effectiveness due to the use of bulk metal instead of nanoparticle-based inks. This approach addresses the challenges associated with current wrap-around electrode designs, including yield, throughput, and cost. The approach of directly prints high-conductivity metal onto the substrate edge, eliminating issues related to photolithography, multi-layer printing, post-sintering, and precise edge shape control. It aims to create wrap-around electrode structures in a scalable, high-throughput process, exploring the interaction between the molten metal and glass to create a crack-free glass-metal interconnect. Key innovations include optimizing conditions for strong metal-to-glass adhesion and the incorporation of a polyimide barrier layer to enhance adhesion. The results show the potential of LMJ to produce highly conductive features for display applications at a significantly lower cost (>50X cost reduction from the material cost standpoint) than existing methods. Future research with focus on improving resolution and expanding the material set to include copper to broaden application needs can enhance the technology's viability.

Biography:

Dr. Manoj Meda is a Sr Research Scientist at Corning Research and Development Corporation. He holds a B.S. in Industrial Engineering from NIT Bhopal, India, an M.S. in Industrial and Systems Engineering, and a Ph.D. in Industrial and Mechanical Engineering from RIT. His doctoral research was focused on fabricating highly conductive flexible electronic circuits at low cost and high throughput using liquid metal jetting. At present, his research interests at Corning Inc, revolve around leveraging digital printing technologies for surface engineering and functional coatings on glass, ceramics, and other substrates using organic and inorganic materials.

Novel Rare-Earth-Free, Tetragonal (L10) Magnets

Ian Baker

Dartmouth College, NH

Abstract:

Demand for high-performance permanent magnets is increasing rapidly for applications such as wind turbine generators and motors in electric and hybrid cars. The rare earth (RE) magnets Sm- Co and Nd-Fe-B magnets are generally used for such challenging applications because they have the highest energy product (BH)max of any material. However, these RE magnets are not without problems such as corrosion and brittle fracture. Other important issues are that over 95% of REs are produced in China, and there has been substantial price volatility of RE elements. Finally, RE mining has been associated with severe environmental degradation. Here we describe research on two tetragonal (L10-structured) low-cost, potentially-commercially-useful permanent magnets NiFe and tau-MnAl that could replace RE magnets. However, there are problems associated with the production of both. The issue for NiFe is that the transformation from the high temperature f.c.c. phase to the L10-structured phase occurs at the equiatomic composition at around 320oC and, thus, is extremely slow. For the metastable phase tau-MnAl, different processing methods have either produced high saturation magnetization or high coercivity but not both simultaneously. In this presentation, we will review previous efforts to produce these magnets and describe our efforts at alloying, based on ab initio calculations, and novel processing (equal channel angular extrusion, electropulse annealing, laser powder bed fusion) to produce the magnets. Funding was provided by the U.S. National Science Foundation (awards CMMI 2039698 and 2032592) and the Irving Institute for Energy and Society at Dartmouth.

Biography:

Ian Baker obtained his BA and D. Phil in Metallurgy and Science of Materials from the University of Oxford. He is the Sherman Fairchild Professor of Engineering and Senior Associate Dean for Research and Graduate programs at the Thayer School of Engineering, Dartmouth College. He is a fellow of ASM, TMS, IOM3, MRS and AAAS. He is co-Editor in Chief of the journal High Entropy Alloys and Materials and Field Chief Editor for the journal Frontiers in Metals and Alloys. He has published over 400 papers and one book entitled “Fifty Materials that Make the World”.

Marangoni migration of rare earth metals during solidification in nuclear fuel rods

Seunguk Mun

Sungkyunkwan University, South Korea

Abstract:

This study identifies a mechanism by which the migration of rare earth metals during the solidification of nuclear fuel rods determines their structure and properties. Nuclear fuel rods are designed to contain a small amount of rare earth metals in a matrix of uranium and zirconium, and the rare earth metals should be uniformly distributed in a fine size. However, rare earth metals have been observed to accumulate near the wall during solidification, and the underlying principle remains unclear. In this study, we employ optical and spectroscopic analysis methods to investigate the phenomenon of rare earth metal particles that form and migrate during the solidification process. A significant difference in surface tension exists between the rare earth metal and the uranium-zirconium medium in the molten state at high temperatures, which induces Marangoni migration, and this possibility is verified by fluid simulation. The results of this study can contribute to a fundamental understanding of the inhomogeneous distribution that occurs during the solidification of metallic materials containing small amounts of rare earth metals and ultimately provide guidance for the development of a uniform distribution while studying the hydrodynamic effects of microstructure inhomogeneity during the transition of alloys from liquid to solid phase.

Biography:

Seunguk Mun is currently a Ph.D. candidate in the Department of Advanced Materials Science and Engineering at Sungkyunkwan university, conducting research on nuclear fuel fabrication, characterization, and simulation. His work focuses on microstructural inhomogeneities and Marangoni-driven segregation in U-Zr-RE alloys, using techniques such as SEM/EDS, XRD, AFM, and fluid dynamics simulations. He is also involved in collaborative research at the University of Utah on non-radiative recombination and photothermal energy conversion in solar thermophotovoltaic systems. His recent interest lies in integrating AI-

based simulation and data analysis methods into nuclear fuel materials development and nuclear fuel design.

Application of Roughness Measurements in Assessing the Resistance of CrN/CrCN Coating and Austenitic Steel to Cavitation Erosion

Alicja Krella

Institute of Fluid-Flow Machinery Polish Academy of Science, Poland

Abstract:

The changes of roughness on the surface of two materials of different stiffness: X6CrNiTi18-10 stainless steel and hard CrN/CrCN multilayer coating during the cavitation erosion test were studied. The coating was deposited using the cathodic arc evaporation PVD method. The structure and mechanical properties of the coating were examined. The erosion tests were performed using a cavitation tunnel. The uncoated steel had no incubation period, in contrast to the CrN/CrCN coating, whose incubation period lasted 45 minutes. The first signs of erosion were the formation of slip bands and deformation twins on the uncoated steel, while indentations formed on the coating, causing it to undulate, as documented by the 3D profiles. The maximum deflection angle of the coating without cracks was about 25o. The volume losses were approximated by straight lines inclined at different angles to the time axis indicating the change in degradation behaviour. The distribution of the Ra parameter on the eroded surface, the maximum value of this parameter (Ramax) and the sum of Ra parameters (∑Ra) from the entire test area were analysed. It was found that material stiffness affected the movement of the location of Ramax during testing time: it remained unchanged on the uncoated steel, whereas on the coating it changed with time. Despite the differences in material properties and volume losses, the Ramax and ∑Ra increased similarly during the initial period of testing. Further behavior of materials under cavitation erosion conditions, the ∑Ra changes revealed better than Ramax.

Biography:

Professor Alicja Krella is the Head of the Centre of Hydrodynamics and Erosion Processes Department at the Institute of Fluid-Flow Machinery Polish Academy of Science, Gdansk, Poland. Since 2021, she is in the World's Top 2% Scientists list compiled by Stanford University and Elsevier. She has published over 80 papers on the subject of cavitation erosion of bulk materials and hard coatings deposited by various methods, including PVD coatings and brush-electroplated coatings. From the beginning of the career, scientific interests were related to mechanics and materials engineering, especially the impact of erosion on fracture behavior.

Plant-mediated Synthesis of Silver-doped Zinc Oxide Nanoparticles and Evaluation of their Antimicrobial Activity Against Bacteria Cause Tooth Decay

Mehran Zareanshahraki

University of Dental Sciences, UCLA, CA

Abstract:

In this research, silver-doped zinc oxide (SdZnO) nanoparticles (NPs) were synthesized in an environmentally friendly manner.

The synthesized NPs were identified by UV–vis spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM). Finally, the antimicrobial activity of synthesized ZnO and SdZnO NPs was performed. It was observed that by doping silver, the size of ZnO NPs was changed. By adding silver to ZnO NPs, the antimicrobial effect of ZnO NPs was improved. Antibacterial test against gram-positive bacterium Streptococcus mutants showed that SdZnO NPs with a low density of silver had higher antibacterial activity than ZnO NPs; Therefore, SdZnO NPs can be used as a new antibacterial agent in medical applications.

Biography:

Mehran Zareanshahraki is a dental professional with 7 years of experience as a dental office manager, specializing in preventive dentistry and implantology. He holds a Mastership in Prosthetic Implant and a Fellowship in Implant Surgery from the International Congress of Oral Implantologists (ICOI). Mehran has extensive experience in electron microscopy techniques, which he applied in both of his research studies to analyze nanomaterials and dental materials at the microscopic level. His publications include studies

on the plant-mediated synthesis of silver-doped zinc oxide nanoparticles for antimicrobial applications and the sealing effectiveness of fissure sealants bonded with universal adhesive systems on saliva- contaminated enamel. He is passionate about integrating green chemistry, nanotechnology, and advanced materials into oral healthcare, contributing to sustainable and innovative dental solutions.

From Prediction to Synthesis: Large Language Models for Accelerating Porous Materials Discovery

Zhiling Zheng

University of California, CA

Abstract:

Large language models (LLMs) are transforming materials research by accelerating data extraction, synthesis planning, and autonomous experimentation. We present an LLM-based framework for metal-organic framework (MOF) discovery that combines text mining, predictive modelling, and multi-agent collaboration. A text-mining agent, built on GPT-3.5/4 with prompt engineering, extracts MOF synthesis conditions from literature with over 90% accuracy, generating a dataset of 26,000 parameters for over 800 MOFs synthesized before. A binary classification model trained on this dataset predicts crystallization outcomes with 87% accuracy, aiding synthetic decision-making. We further introduce the ChatGPT Research Group, a team of LLM-powered agents that coordinate tasks such as literature review, code generation, and robotic control. This system autonomously discovers synthesis conditions for two new pyraozole- and thiophene-based water-harvesting MOFs, respectively, using Bayesian optimization and reasoning. Our results demonstrate that LLM agents have potential of boosting research productivity and serve as powerful collaborators in experimental materials science.

Biography:

Zhiling Zheng is a Postdoctoral Fellow at BIDMaP Institute, UC Berkeley, and incoming Assistant Professor of Chemistry at Washington University in St. Louis. He completed postdoctoral research at MIT with Professor Klavs F. Jensen and earned his Ph.D. in Chemistry from UC Berkeley in 2023 under Professor Omar M. Yaghi. Previously, he received his B.A. degree from Cornell University in 2019. Dr. Zheng's research has focused on designing metal-organic frameworks (MOFs) for atmospheric water harvesting. Beyond experimental work, he also explores large language models (LLMs) for data mining, reaction and material design, and synthesis planning, aiming to advance AI-driven chemical research.

Cluster-based Energy Materials – A Paradigm shift in Design and Synthesis

Puru Jena

Virginia Commonwealth University, VA

Abstract:

Although the Periodic Table of elements is the mother of all materials, it has limitations; the number of elements is fixed, their chemistry is pre-determined and cannot be altered, and some of them are either rare or toxic. Atomic clusters, composed of a few to a few thousand atoms, provide a way to overcome these limitations, because their chemistry can be tailored by customizing their size, composition, symmetry, and charge state. This talk will deal with the rational design of these super atomic clusters [1] that not only mimic the chemistry of atoms but also can be assembled to form bulk materials with properties superior to those of conventional atom-assembled materials. The examples will include super atomic clusters that promote unusual reactions such as making noble gas atoms form chemical bonds at room temperature [2], activate gas molecules such as CO2 [3], and form the building blocks of all solid-state Li-ion batteries with high ionic conductivity and interfacial stability [4-6]. These results based on multi-scale first principles theory are validated by experiments.

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on cluster ions", Proc. Nat. Acad. Sci. 14, 1047 (2017) [6] Fang, H., Jena, P.: "Argyrodite-type advanced lithium conductors and transport mechanisms beyond paddle-wheel effect", Nature communications 13 (1), 1-11 (2022) 10.1038/s41467-022-29769-5

Electrocaloric and elastocaloric effects in soft materials

Brigita Rozic

Jožef Stefan Institute, Slovenia

Abstract:

Phase-changing materials with large caloric effects have the promise of realizing solid-state refrigeration, which is more efficient and environmentally friendly than current techniques [1]. A review of recent direct measurements of the large electrocaloric effect in liquid crystalline materials and the large elastocaloric effect in liquid crystal elastomers will be given [2,3]. The large electrically induced multicaloric effect exploiting both orientational nematic and positional smectic energy reservoirs was found near the isotropic phase transition in liquid crystalline materials and mixtures of liquid crystals with functionalized nanoparticles. Direct measurements indicate that the large elastocaloric response with giant elastocaloric responsivity can be found in main-chain liquid crystalline elastomers. Both soft materials can play a significant role as active cooling elements and parts of thermal diodes or regeneration materials in developing new cooling devices. [1] Z. Kutnjak., B. Rozic. and R. Pirc., Electrocaloric Effect: Theory, Measurements, and Applications (Wiley Encyclopedia of Electrical and Electronics Engineering) 2015, p. 1-19. [2] D. Črešnar et al, J. Phys. Energy 5: 045004, 2023. [3] A. Rešetič et al, Nat Comm 7: 13140, 2016.

Structure-property relationships of nanostructured materials: from synthesis to characterization for multiple applications

Sara Cerra

Sapienza University of Rome, Italy

Abstract:

Materials in the nanoscale range exhibit fascinating properties compared to their bulk counterparts, i.e.,light absorption and scattering, high surface-to-volume ratio, surface reactivity, electrical, and magnetic properties. Among these, functionalized noble metal (MNPs), metal oxide (MOxNPs), polymeric nanoparticles (PNPs) and related hybrid organic/inorganic nanocomposites depict a suitable platform for developing multi-functional responsive systems with applications in nanomedicine, sensing, and optoelectronics [1-5]. Plasmonic nanoparticles, i.e., gold, silver, and palladium nanoparticles (AuNPs, AgNPs, PdNPs), and metal oxide nanoparticles (TiO2NPs, Fe2O3NPs) bear several advantages: tunable size, ease of surface functionalization, and colloidal stability. Exploring different hard and soft surface chemistry, different stabilizing agents-commercial or synthetic – were used to functionalize the nanoparticles surface, also tuning their interfacial properties. Different surface functionalities were explored using negatively and positively charged ligands to obtain nanoparticles with single or mixed functionalities. Using bifunctional organic and organometallic ligands their 2D or 3D can be manipulated to induce self-assembly into covalent networks with collective properties. Extensive physicochemical characterizations were carried out to determine the nanoparticles characteristics including their size, shape, surface morphology, surface charge, structure, stability, and optical properties for applicative purposes.

Biography:

Dr. Sara Cerra completed her PhD in Chemical Sciences in 2022 at Sapienza University of Rome. Currently she is a post-doctoral research fellow at Sapienza University of Rome focusing on the synthesis and characterization of noble metal, metal oxide, and polymeric nanoparticles functionalized with hydrophilic, hydrophobic ligands and organometallic acetylide complexes, with the aim to exploit the structure- properties correlations and physicochemical properties of nanomaterials. She is also involved in applicative studies in the field of optoelectronics, sensing, nanomedicine, and biotechnology in collaboration with national and international research groups. She is author of 26 peer-reviewed papers, H-index: 8.

Conservation of energy and momentum of drifting electrons in materials

Ravi Kumar Chanana

Self-Employed Independent Researcher, India

Abstract:

Conservation of energy and momentum of free electrons in all materials is expressed in the equation form as: $\frac{dE}{E} = \frac{dp}{p} = \frac{dm}{m}$ for drifting electrons in materials at constant velocity at a high electric field in KV/cm. The energy of the free electrons in all materials (metals, insulators, semiconductors) is expressed by the equation: $\frac{1}{2} m_{eff} v_{th}^2 = \frac{3}{2} kT$ as given in the reference [1] below. In semiconductors and insulators, the drift velocity is of the same order as the thermal velocity of about 105 meters/sec, but in metals the drift velocity is much slower of the order of 10-4 meters/sec. The density of free electrons is of the order of 1022/cm3 in metals as compared to those in high resistivity semiconductors of the order of 1014/cm3. This causes more collisions of electrons with the lattice atoms and defects in metals reducing the drift velocity of the free electrons. Just to mention, the above laws of conservation of energy and momentum are associated with the inertial frame of drifting electrons at constant velocity in materials as the symmetry of nature where the laws of physics do not change, thus asserting Noether's theorem. Also, dE/E = dm/m can also explain a burning star where change in energy results in change in mass of the star. A corrective suggestion by Dist. Prof. Emeritus, Physics & Astronomy and Mats. Sc. and Engg., Leonard C. Feldman at Rutgers State U. in New Jersey, USA, is acknowledged.

Biography:

I, Ravi Kumar Chanana, am a retired Professor of Electrical and Electronics Engineering. I taught for 15 years in India and did research as a Scientist in the field of MOS Physics and Technology for more than 33 years since 1989, publishing more than 115 research papers in International and National Journals and Conferences. I completed B.E. (Hons.) degree in EEE from BITS, Pilani, India in 1981, M.S. degree with thesis, in EE from U. of Louisville, KY USA in 1984, and Ph.D degree in EEE from Institute of Technology, BHU, Varanasi, India in 1992. I also did post-doctoral research in USA for about 3.5 years from April 1997 to December 2000 in the Metal-Oxide-Semiconductor (MOS) research area at UAB, Birmingham, AL, and Vanderbilt U., Nashville, TN. USA.

The Effect Of Soybeans Hull (Glycine Max), Beans Pod (Phaseolus Vulgaris) And Dry Willow Leaf (Salix Spp) On The Properties Of A Simple Water -Based Mud

Sarah A. Akintola

University of Ibadan, Nigeria

Abstract:

Agro-waste materials, instead of being disposed, can find valuable applications in the oil and gas industry as drilling fluid additive. This study is aimed at investigation of the effects of temperature and aging time on the property of a water-based mud treated with soybean hull, beans pod and dry willow leaf. The agro waste were proficiently sun-dried, pulverized and sieved into fine powder then stored in an air tight labelled container. The recommended API 13A-1 procedure was used in the determination of the rheology and filtration properties of the mud samples treated with the additives at varying concentration (2g, 4g, 6g, 8g and 10g) at temperatures of 80°F, 140°F and 194°F were determined with samples treated with CMC used as control. From the result, it was observed that the mud samples containing soybeans have the highest plastic viscosity with those with dry willow leaf the highest yield point. The effect of aging on the mud sample shows the plastic viscosity of each of the mud sample decreased with soybeans having the highest plastic viscosity. While the yield point and gel strength at 10 minutes and 10 seconds increased respectively with dry willow leaf having the highest yield point. The result of the fluid loss shows the mud samples treated with dry willow exhibiting the closet linear relationship with sample treated with CMC at room temperature, but as temperature increased samples with beans pod exhibited the closet linear relationship with that of the control.

Biography:

Sarah A.Akintola is a lecturer at the department of Petroleum Engineering, University of Ibadan, Ibadan. Her research activities are in the area of Polymer-based Materials as drilling fluids additive, Drilling Fluid Chemistry, Corrosion Engineering, and Well Engineering.

Metal-insulator Transition in Bulk Ge2 Sb2 Te(5-5x) Se5x Phase Change Materials

Utpal Chatterjee

University of Virginia, VA

Abstract:

Phase Change Materials (PCMs) are well-known for their reversible yet swift switching between crystal-to-amorphous transition (CAT) through Joule heating at the presence of electric or laser pulses. This CAT is also followed by a metal-to-insulator transition (MIT), whose mechanism remains unresolved despite decades of study. The spectacular contrast in physical properties of these materials across the CAT makes them suitable for futuristic memory and optoelectronic applications. Ge2Sb2Te5 (GST) is one of the most studied PCMs. The optimization of various material properties, e.g., the rate of crystallization, thermal stability, and the enhancement in the change of electrical resistivity across MIT, are critical to the widespread integration of GST in device architectures. Recent studies suggest that Ge2Sb2Te(5-5x)Se5x (GSST), i.e, Se doped GST, could potentially resolve some of these pressing material issues since GSST offer (i) lower crystalline temperature and (ii) higher contrast between electrical resistivities during MIT across the CAT. Combining spectroscopic measurements via Angle Resolved Photoemission Spectroscopy (ARPES), and electrical as well as magneto transport measurements we studied the MIT in a series of GSST bulk samples. Our studies evidence the significance of electronic inhomogeneity and the possible existence of multiple mobility edges in the vicinity of the MIT in GSST.

Biography:

Utpal Chatterjee is an associate professor at the physics department of the university of Virginia (UVA). He Joined UVA in 2012. Before joining UVA, he was a director's postdoctoral fellow at the Materials Science Division of Argonne national lab. He did his PhD is from the University of Illinois at Chicago in December 2007. His research interest lies in the experimental investigations of various functional materials which have bearings to practical applications and exhibit novel electronic phenomena at the same time. Examples include cuprate high temperature superconductors, transition metal dichalcogenides hosting intriguing interplay between charge density wave (CDW) and superconductivity and several narrow band gap semiconductors displaying unique topological and thermoelectric properties. For the experimental studies, he employs a combination of experimental probes, which include Angle Resolved Photoemission Spectroscopy (ARPES), electrical and magnetic transport and Raman Scattering experiments.

Thermoelectric Properties of Graphene Nanoplatelets and Organic Semiconductor Composites

Andrea Reale

University of Rome Tor Vergata, Italy

Abstract:

Thermoelectric (TE) materials are considered the most preferable materials in recent technology for harvesting waste heat into electrical energy. However, high-temperature fabrication process, brittle nature, possible harmful concerns of inorganic TE materials, limit a widespread application. In the recent decade, composites of organic polymers like PEDOT and P3HT with carbon base nanostructures like graphene nanoplatelets (GNP) and carbon nanotubes (CNT) have gained much attention as TE materials for energy harvesting applications. Herein, a novel processing approach will be applied to fabricate TE devices using P3HT and GNP nanocomposites. The role of GNP:P3HT concentration and the type of P3HT dopants are discussed. Different deposition techniques will be considered, such as blade coating for planar device layout, and pellets for 3D device layout, measuring TE effects (Seebeck coefficient, Power factor, electrical conductivity) in different configurations of heat flow through the active TE material. Possible module layouts will be also discussed.

Biography:

Research activity of Prof. Reale (H=40, Google Scholar) is focussed on 1) Printable electronics for energy: development and characterization of devices based on organic semiconductors and organic-inorganic hybrids, with particular attention to the technological aspects of large-area scale-up for applications in the energy field (photovoltaic, thermoelectric, termoelectrogalvanic) and telecommunication devices (photodetectors for VLC and IR, IR sources); 2) Nanostructured materials (graphene, carbon nanotubes): study of technological applications (thermoelectric composites, thermal management, deformation sen-

sors); 3) Theoretical and experimental analysis of the optical, electro-optical and electrical properties of heterostructure devices for electronics and telecommunications.

Exascale Transport Simulations for the Understanding of the Switching Mechanism in Atomically Thin Memristors

Liangbo Liang

Oak Ridge National Laboratory, TN

Abstract:

Non-volatile resistive switching (NVRS) has emerged as an important concept in the development of high-density information storage and computing. The recent discovery of NVRS in two-dimensional (2D) monolayer structures, such as MoS2 and hexagonal boron nitride (hBN), open a new avenue for memory/computing devices at the ultrathin scale. The fundamental switching mechanism in 2D monolayers, however, is not yet fully understood. It is hypothesized that vacancies in 2D monolayers mediate formation of conducting filamentary channels leading to a high- to low resistance state. But to fully unravel the switching mechanism, it is highly desirable to simulate the electronic transport in a realistic device geometry using ab initio approaches for comparison with experimental data. This is a rather challenging task as quantum transport simulations are computationally demanding. Here, for the first time, we report results from simulations of electronic transport of ~1000 atom systems consisting of a hBN monolayer sandwiched by top and bottom gold electrodes and compute I-V curves. These large quantum transport simulations are made possible by implementing the non- equilibrium Green's function (NEGF) method in a highly scalable first-principles DFT code: the Real-space MultiGrid (RMG) that runs efficiently in the first exascale supercomputer, Frontier, at Oak Ridge National Laboratory. Systematic NEGF calculations uncover that experimental devices exhibit a wide range of current ON/OFF ratios owing to the varied interface spacing between the electrode surface and hBN and provide a deeper understanding of the resistive switching mechanism in atomically thin memristors.

Biography:

Dr. Liangbo Liang is a research staff member in the Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL). His current research lies in condensed matter theory and computational physics, focusing on developing and applying large-scale theoretical/computational methods on supercomputers to understand and engineer diverse materials from first principles. Methods including density functional theory and many-body GW approach are used to study electronic, magnetic, optical, vibrational, and Raman scattering properties of quantum materials and nanomaterials such as carbon nanotubes, graphene, transition metal dichalcogenides, metal halides, black phosphorus, etc.

Reducing Enzyme and Bacterial Activity in Diabetic Ulcers with WAAPV-infused Electrospun Fibers

Helena Prado Felgueiras

University of Minho, Portugal

Abstract:

Diabetic ulcers are often worsened by elevated levels of human neutrophil elastase (HNE) and bacterial infections, both of which impede healing. To address these challenges, polycaprolactone (PCL)/polyethylene glycol (PEG) electrospun fibers infused with elastase- targeting peptides, AAPV and WAAPV, were engineered. Fibers were designed to exert multiple actions, including inhibiting HNE. WAAPV's effectiveness in regulating proteolytic enzymes was verified by its ability in inhibiting HNE activity. The incorporation of PEG into the fibers enhanced their wettability, although it also accelerated degradation. However, the inclusion of WAAPV mitigated this effect, resulting in a sustained release of peptides over 24 hours. Peptide loading within the fibers was confirmed through thermal stability and hydration capacity analyses, and the peptide concentrations were determined by mass/dimension ratios in approximately 51.1 μg/cm2 and 46.0 μg/cm2 for AAPV, and 48.5 μg/cm2 and 51.3 μg/cm2 for WAAPV, within PCL and PCL/PEG matrices, respectively. Both peptides effectively inhibited HNE, with PEG showing potential to enhance this inhibition by interacting with the peptides and forming peptide-PEG complexes. The fibers containing PCL and peptides achieved approximately 10% HNE inhibition after 6 hours of incubation, while PCL/PEG fibers showed ≈ 20% inhibition after 4 hours testing. Peptide-loaded fibers demonstrated significant antibacterial activity, inhibiting the growth of Staphylococcus aureus by up to 78% and Escherichia coli by up to 66%, with peak

efficacy observed after 4 and 2 hours of incubation, respectively. These findings suggest that WAAPV-loaded fibers hold promise for inhibiting HNE and bacterial activity, and thus for treating diabetic ulcers.

Biography:

Dr. Helena Felgueiras (HF) is a Biomedical Engineer with a PhD also in Biomedical Engineering (University Paris 13, 2014). Her work focuses on biomedical surface functionalization and the microbiology of biomaterials. She has developed surfaces for bone repair and chronic wound treatment using bioactive molecules. HF is an Auxiliary Researcher at 2C2t, and has authored 57 articles, 7 book chapters, and 1 book, with an h-index of 24. HF has 154 communications and collaborations across >10 countries and 13 projects. She has supervised the work of >30 researchers. In 2023, she was among the "World's Top 2% Scientists" (Stanford/Elsevier).

Study of Radio-frequency Epsilon-negative Behavior in LaNiO3 for Microwave Shielding Applications

Tarun Katheriya

Indian Institute of Technology (BHU) Varanasi, India

Abstract:

This study investigates the radio-frequency epsilon-negative behaviour in nanostructured LaNiO3 and develop a modified approach to explain this behavior and explores its potential applications in electromagnetic interference (EMI) shielding and stealth technologies. We synthesized a LaNiO3 using the sol-gel method, owing to its metallic conductivity, which is a prerequisite for effective shielding phenomena. The x-ray diffraction studies have confirmed its rhombohedra structure and, electrical characterization demonstrated a consistent trend of epsilon negative behavior (~1.2x107), and metallic conductivity (~130 S.m-1) across the entire frequency spectrum (100 Hz-1.5 MHz) and up to 100 °C. We applied the Drude model and extended it by incorporating additional interaction terms to explain the observed negative permittivity behavior for single-phase material. Our extended model attributes this behavior to the plasmonic oscillation of delocalized free carriers. By fitting this modified Drude model, we were able to calculate key parameters such as plasma frequencies (ωp) and damping frequencies ($\omega \tau$). The results indicate that the low plasma frequency is due to a combination of low carrier density and an increased effective mass, which arise from strong electron-electron interactions. Furthermore, the temperature dependence of the DC conductivity suggests that small-polaron hopping mechanisms contribute to the observed conductivity behavior. Impedance studies have confirmed that the inductive behavior observed is an inherent property of LaNiO3. Microwave shielding studies have demonstrated good shielding capabilities at room temperature, with shielding effectiveness of approximately -33 dB, attributed to reflection as the dominant phenomenon. These findings underline the potential of LaNiO3 for various applications such as coil-less inductors, microwave shielding materials, and circuit miniaturization.

Impact of Hyperglycemia on Glioblastoma Cell Proliferation and the Therapeutic Potential of Green-synthesized CeO2 NPs

Sohail

Yangzhou University, China

Abstract:

The diabetes mellitus is a risky factor for cancer patients including malignant glioblastoma. The complications arise due to hyperglycemia along with glioblastoma (GB) cancer cells behavior are still not clear. The results of the given research disclose that high glucose promoted the cell division and proliferation of glioblastoma cell line U87. Glioblastoma cancer cells were cultured in 5 mmol/L, 10 mmol/L, and 25 mmol/L of glucose and treated with three different CeO2NPs for different time intervals. The cytotoxicity results elucidate that CeO2NPs invasion in glioblastoma cancer cells cause losing selective membrane potential, prevent the synthesis of myofibroblast, and elevate the reactive oxygen species (ROS) generation in cancer cells. In the following experimental work, the anticancer potential of green CeO2NPs was explored using new powerful techniques including cytotoxicity assay, nuclear apoptosis assay, and mitochondrial degradation assay. The variable oxidation state and electropositive nature of CeO2NPs cause oxidation of chromatin material. The confocal microscopic results make clear invasion of CeO2NPs inside the nucleus

and apoptotic cells look like star shape. Mitochondrial degradation potential of three different green synthesized CeO2NPs was checked against glioblastoma U87 cancer cells. CeO2NPs invade in the inner mitochondrial membrane cause breakdown of electron transport chain (ETC) and release oxidative radicals throughout the cell which accelerate the pathway of oxidation of subcellular organelles. Hence, our study revealed that high glucose promotes the glioblastoma cancer cells multiplication and progression. The breakdown of ETC resultant no more ATP production and halt cancer cell metabolism. The green CeO2NPs penetrate in nucleus and integrate with chromatin material of glioblastoma cancer cells resultant denaturation of genetic material. Green CeO2NPs were found effective to cross the subcellular membranes and halt cell division and glucose metabolism, destroying nucleus and mitochondria of cancer cells.

Poster Presentations

Alternative Wire Manufacturing Technology from Titanium and Nickel Shavings

Michal Duchek

COMTES FHT a.s., Czech Republic

Abstract:

This study presents an alternative method for manufacturing titanium and nickel wires from recycled machining shavings using a Continuous Extrusion Machine (Conform process). This innovative approach eliminates the need for energy-intensive multi-step remelting, which is traditionally required for wire production from metallic chips. The continuous extrusion process enhances material efficiency, reduces energy consumption, and minimizes waste. The key to achieving high-quality wire lies in the precise preparation and compaction of the shavings into feedstock suitable for direct processing in the Conform Machine. The study evaluates the influence of feedstock properties on the resulting wire's mechanical and structural characteristics.

Biography:

Michal Duchek (born November 17, 1980, Czech Republic) is a metallurgical engineer specializing in materials engineering and engineering metallurgy. He earned his M.Sc. in Metallurgical Engineering from the University of West Bohemia, focusing on FeNi alloys for his diploma thesis. Since 2016, he has been heading the Metallurgical Technologies Department at COMTES FHT a.s., where he oversees research and development in advanced metallurgical processes. His contributions have played a key role in the advancement of metallurgical engineering, reflected in his participation in numerous research projects, as well as his authorship of patents

Evaluating the Corrosion Resistance of Nickel-Based Superalloys in Fluoride Salts for Molten Salt Reactors

Pavel Podaný

COMTES FHT a.s., Czech Republic

Abstract:

The study examines the corrosion behavior of the MONICR alloy in molten fluoride salts (FLiBe and FLiNaK) under conditions relevant to molten salt reactors. Corrosion tests at 650–700°C for up to 750 hours demonstrated that MONICR has superior resistance compared to other tested alloys, including INCONEL 625, Alloy 800 HT, AISI 304, AISI 321, HASTELLOY N, and GH355. Microstructural analysis revealed chromium and molybdenum depletion near the surface, increased nickel concentration, and the formation of sulfur-rich particles. Corrosion predominantly occurred at grain boundaries but avoided twin boundaries. These results highlight MONICR's potential for high-performance applications in molten salt reactors.

Biography:

- Pavel Podaný - Ph.D. in Materials Science from the University of West Bohemia.

- Authored/co-authored over 40 scientific papers in Web of Science and 68 in Scopus, with a Researcher ID of R-1921-2017 and ORCID: 58111194500.

- Presented at over 30 international and domestic conferences, contributing significantly to the field of materials science.

- Inventor/co-inventor of over 30 technologies for metallic materials processing and a patent for eco-friendly machinable brass.

- Served as coordinator/contact person for research projects funded by prestigious agencies, including EUREKA, Czech Science Foundation, Ministry of Industry and Trade of Czech Republic etc.

Effect of the laser cleaning method on the corrosion resistance of Mg alloy AZ80

Frantisek Novy

University of Žilina, Slovak Republic

Abstract:

Magnesium alloys are the lightest structural metallic materials, which are widely used in automotive industry, aerospace, military, biomedicine and other fields, but their poor corrosion resistance remains a significant drawback, that diminishes their usage in various industrial branches. Therefore, it is necessary to improve their insufficient corrosion resistance by appropriate surface treatment techniques including PVD, fluoride-based coatings, electrochemical plating, laser cladding, anodizing or plasma electrolytic oxidation (PEO). PEO process allows the formation of thick and adherent ceramic like coatings on various types of metals, including magnesium alloys. Unfortunately, the obtained coating resulted in richness of pores and cracks on the surface, which form pathways for aggressive medium impairing the protective effect of PEO. To reduce the porosity of the coating, different surface pre-treatments for the PEO coatings were performed in literature: grinding, polishing and shot peening. In order to improve the corrosion resistance and reduce the porosity of PEO coatings applied on magnesium alloy AZ80, a laser cleaning method was used before the PEO process as a pre-treatment step. Corrosion resistance of prepared coatings was analyzed by using potentiodynamic polarization tests (PDP) at the laboratory temperature in 0.1 M NaCl water solution. Additionally, roughness measurements were performed to assess the effect of the pulsed laser on the surface of the base material prior to PEO process. Results showed that pre-treatment by laser decreased corrosion stability of PEO coating due to the local presence of oxides on the surfaces which impeded growth of the coating in these locations.

Biography:

Prof. František Nový graduated from the Faculty of Mechanical Engineering of the University of Žilina, Slovak Republic in 1996 and defended his PhD in 2002. Since 1996, is working at the Department of Materials Engineering and in 2022 he became a full professor at university of Žilina. In the field of Materials engineering, Physical metallurgy of metallic materials and Surface engineering he deals with the evaluation of the mechanical properties and degradation mechanisms of the structural materials, especially evaluation of effects of various surface treatments on the fatigue and corrosion endurance of dynamically loaded components of mechanisms and structures.

Comparative Study of Bond Behavior of BFRP and GFRP Bars in Concrete Modified with Metakaolin and Zeolite Using Beam and Pull-Out Tests

Julita Krassowska

Bialystok University of Technology, Poland

Abstract:

This study explores the impact of metakaolin and zeolite additives on the bond strength between fiber-reinforced polymer (FRP) bars and concrete, comparing the results from beam and pull-out tests. The beam tests revealed a significant reduction in bond stress for BFRP bars, with a 35% and 40% decrease when using metakaolin and zeolite, respectively, compared to steel bars. In contrast, the pull-out tests showed bond stresses up to three times higher for BFRP bars in reference concrete. The pull-out tests apply direct tension to the bars, resulting in high bond stresses, while the beam tests simulate more complex real-world stress conditions, such as bending and shear. The study suggests that although metakaolin and zeolite improve the microstructure of concrete, they may lower bond stress values compared to traditional concrete, particularly under complex stress states. These findings emphasize the need for tailored design approaches to accurately evaluate and optimize the bond performance of FRP bars in concrete, considering the differences revealed by the varying test methods.

Biography:

Main interests include innovative building materials, particularly concrete with basalt fibers, applications of cement composites in infrastructure constructions, and technologies for the production of prefabricated concrete elements.

Characteristics of Recycled Carbon Fibers Used for Concrete Reinforcement

Malgorzata Gradzka-Dahlke

Bialystok University of Technology, Poland

Abstract:

The pursuit of "green energy" has led to the development of wind power plants. However, wind turbines have a limited lifespan, which necessitates the disposal of the materials used in their construction. This has sparked growing interest in the possibility of recycling these materials. Recovered materials, such as carbon fibers, can be repurposed in construction, automotive, and aviation industries, granting them a second life and increasing their economic value. The use of fibers in concrete structural elements enhances crack resistance, mitigates shrinkage cracking, and prevents brittle failure of concrete. This article presents the characteristics of carbon fibers recycled from wind turbine blades, including microscopic observations and mechanical property testing. Additionally, the study examines the effect of adding these fibers to concrete reinforcement. Mechanical properties of concrete with fiber additions were tested, and microscopic observations were conducted. The results demonstrated a significant improvement in the flexural strength of concrete compared to concrete without carbon fiber addition. Observations indicated a very favorable distribution of carbon fibers in the concrete. Bundles of long fibers enhanced the material's strength, while randomly distributed individual fibers counteracted crack propagation in the concrete. The study also confirmed good adhesion of the fibers to the concrete matrix. The findings underscore the potential application of recycled carbon fibers in practical construction, contributing to sustainable development within the construction sector. The work was carried out at the Bialystok University of Technology. Project supported by the Ministry of Science in the frame of „Regional Initiative of Excellence".

Biography:

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Multi-Scale Analysis of Fracture Processes in Concrete with Basalt Fiber Reinforcement

Marta Kosior-Kazberuk

Bialystok University of Technology, Poland

Abstract:

This study investigates the fracture processes in concrete reinforced with basalt fiber and basalt fiber-reinforced polymer (BFRP) bars, focusing on bending and shear behavior. A total of 24 beams (0.12×0.3×4.5 m) with various types of longitudinal reinforcement and different stirrup spacings were analyzed, including reference beams reinforced with steel bars. The test results revealed that the addition of basalt fibers increased the shear capacity by an average of 20% in both series. However, beams with BFRP reinforcement exhibited up to 26% lower shear capacity compared to steel-reinforced beams. The inclusion of basalt fibers also altered failure modes, transitioning from brittle web shear crushing to more ductile shear-flexural failures, improving crack resistance, enhancing crack distribution, and increasing the energy required for failure. These findings highlight the potential of basalt fibers and BFRP bars to enhance the structural performance and durability of concrete, offering a promising solution for sustainable construction applications.

Biography:

Since 2020, Marta Kosior-Kazberuk has served as the Rector of Bialystok University of Technology and is

currently the Head of the Department of Construction and Building Mechanics. Her research focuses on the durability of concrete structures, the effects of mineral additives on concrete, and the protection of capillary-porous materials.

Impact of Aluminium Content on Structure and Mechanical Properties of AlxCoCrFeNi High-Entropy Alloys

Malgorzata Gradzka-Dahlke

Bialystok University of Technology, Poland

Abstract:

High-entropy alloys (HEAs) have been a focus of research for nearly two decades due to their potential for unique mechanical and functional properties. By adjusting alloying elements and heat treatments, these properties can be tailored for diverse applications. Among HEAs, AlxCoCrFeNi stands out, with aluminum content playing a critical role due to differences in atomic radii. Understanding the strengthening mechanisms of these materials is a key research objective.

This study investigates the influence of aluminum content on the microstructure and mechanical properties of AlxCoCrFeNi alloys. Materials were produced by induction melting of pure metals in an argon atmosphere. X-ray diffraction (XRD) revealed that the crystal structure evolves with aluminum content. At x=0, the alloy exhibited a homogeneous solid solution crystallizing in the FCC system. As aluminum content increased, a BCC phase appeared and grew in proportion. Microstructural analysis confirmed these changes. The x=0 alloy displayed a uniform structure without phase separations. At x=0.5, dendrites formed, consisting of solid solutions of alloying elements, with a phase mixture visible in interdendritic spaces. Higher aluminum content led to increased phase segregation. Mechanical properties varied significantly with aluminum content. Increased aluminum resulted in higher tensile strength and hardness, but reduced ductility. Samples maintained high ductility up to x=0.7, while x=1 exhibited brittle fracture. These results indicate that both solution strengthening and microstructure influence the mechanical properties of AlxCoCrFeNi alloys.

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Biography:

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