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University of Toronto

Contents

Plenary Talks

Towards Managing Advanced Steel Surface Chemistries in Continuous Annealing and Galvanizing

Joseph McDermid

McMaster University

Metal Chemistry Lecture

Abstract:
The world-wide cost of corrosion estimated at approximately $2.5 trillion USD per year, a significant portion of which can be assigned to the corrosion of ferrous materials. This cost is significantly mitigated, however, through galvanizing, in which a thin layer of Zn applied to the steel surface such that it sacrificially protects the underlying steel from aqueous corrosion. Globally, almost 350 Mt/year of sheet steel are galvanized, making it one of the most important technologies deployed to manage the costs of corrosion. In addition, the extension of product and infrastructure lifetimes provided by the corrosion prevention of steel through galvanizing has kept millions of tons of carbon dioxide from being emitted in replacement steel production.

More recently, significant vehicle mass reductions have been realized through the increased deployment of Zn-coated advanced high strength steels (AHSSs) in advanced automotive architectures. This dramatic change has led to significant safety and fuel efficiency improvements in conventional vehicles and is a key enabler to the deployment of the next generation of electric vehicles. Increases in AHSS properties have typically come through more highly alloyed steel chemistries coupled with sophisticated thermal processing routes and part geometries employing thinner material cross-sections – for which robust corrosion protection provided through galvanizing is essential to maintain vehicle safety.

However, the increased levels of alloying elements have resulted in complex surface chemistries and significant challenges with respect to the production of high-quality Zn-based coatings. This paper will discuss the fundamental challenges of deploying Zn-coated advanced steels into automotive structures, with a focus on gas/metal reaction thermodynamics and kinetics, the resultant surface chemistries and how these can be beneficially altered through various processing strategies ensuring that the required reactions with the zinc alloy bath take place.

Atomistic processes of deformation in nanocrystals with in-situ high resolution transmission electron microscope

Scott X Mao

University of Pittsburgh

Metal Physics Lecture

Abstract:
Competition between different deformation mechanisms in nanoscale materials determines their plastic behaviours. Here, by in-situ high resolution transmission electron microscopy (HRTEM) observation, the competition of interior deformation mechanisms in nanocrystals were revealed. It was found the competition between the emission of leading partials and trailing partials from surface led to the transition between dislocation slip and twinning in gold nanocrystals. The orientation-dependent plasticity was also observed in body-centered cubic tungsten nanowires. Twinning-dominated plastic behaviour and discrete shear-band plasticity in tungsten nanowires were found, which was contributed to the competition between twinning and dislocation-slip under different loading orientation. In addition, an interesting deformation model, diffusional creep, different with the dislocation-slip and twinning, was demonstrated to play an important role on the plasticity in nanowires at room temperature. The surface-creep activated by dislocation-slip could lead to a super-elongation in silver nanocrystals with certain range sample diameters while the dislocation slip would dominate the deformation beyond the range. These works advance understanding of the competition and transition among dislocation slip, twinning and surface diffusional creep, which provides guidelines to optimize the mechanical performances of metallic nanocrystals in application.

Electrochemical Pathways Towards Deep Decarbonization and Profitable Sustainability

Donald R. Sadoway

Massachusetts Institute of Technology

D.K.C. MacDonald Lecture

Abstract:

A sustainable future is axiomatically a carbon-free electric future. Emerging technologies that will usher in this new economy necessarily include electrochemical innovations in energy storage and in steelmaking. Electricity storage is critical to widespread deployment of carbon-free but intermittent renewables, solar and wind, while offering huge benefits to today's grid: improving security and reducing price volatility. Invented at MIT, the liquid metal battery provides colossal power capability on demand and long service lifetime at very low cost and without threat of fire. In 2019 worldwide steel production generated 9% of total CO2 emissions. Invented at MIT, molten oxide electrolysis represents an environmentally sound alternative to today's carbon-intensive thermochemical process. Instead of CO2 as the by-product of steel, molten oxide electrolysis makes tonnage oxygen while offering better metal at lower cost while vitiating negative environmental impacts of current technology. In the narratives of both of these emerging technologies, liquid metal battery and molten oxide electrolysis, there are lessons more broadly applicable to innovation: how to pose the right question, how to engage young minds (not experts), establishing a creative culture, and inventing inventors in parallel with inventing technology.

2D Materials

Oral presentations:

High Cycle Wear Behavior of 2D Materials

Nima Barri, Md Akibul Islam, Li Ma, Pedro Guerra Demingos, Boran Kumral, Chul B. Park, Chandra Veer Singh, Tobin Filleter

University of Toronto

Abstract:

Wear plays a crucial role in determining the lifetime and reliability of nanoscale mechanical systems with moving parts. Understanding this phenomenon at the nanoscale is of great importance for applications such as nanolithography and nanomanufacturing. Because of the complicated nature of nanoscale wear, the behavior of two-dimensional materials under high cyclic wear and their surface damage mechanism is yet unknown. In this study, by employing atomic force microscopy-based scratch testing and molecular dynamics simulations, high cycle wear behavior of a single layer graphene, MoS2, and Ti3C2Tx (MXene) has been investigated. High cycle wear experiments have been conducted using a sharp diamond tip scratching over a single line in a reciprocating manner. At 85% of the applied critical normal load (the minimum load at which the material fails instantly and exposes the substrate under a single cycle), graphene sustained superlubricity for more than 3000 cycles before failure, followed by MoS2 and Ti3C2Tx, which failed at the average of 500 and 50 cycles, respectively. High cycle wear failure in monolayer graphene and MoS2 is almost catastrophic with minimal progressive damage. On the contrary, Ti3C2Tx showed progressive damage before failure, mostly due to the presence of surface termination groups. The findings on the failure mechanism and long-term high cycle wear endurance are crucial to designing reliable coating layers for nanoscale devices.

Correlative Electron Microscopy of Van der Waals Heterostructures

Nabil Bassim

McMaster University

Abstract:

Recently, the synthesis of various 2D materials confined at the epitaxial graphene/SiC interface has been realized through confinement heteroepitaxy (CHet). In this technique, atoms intercalate at the interface of epitaxial graphene (EG) and silicon carbide (SiC) substrates via a thermal evaporation process, typically at 800 °C. While the EG is deliberately damaged using plasma to open intercalation holes prior to the CHet process, the EG is found to be healed after the metal intercalation due to a metal catalytic effect. The CHet process facilitates scalable and environmentally air-stable 2D metals and alloys over millimeter-scale. CHet metals and alloys exhibit novel properties, such as enormous second harmonic generation, superconductivity, and epsilon-near-zero behavior. Understanding the atomic structure of these van der Waals heterostructures yields insights into their growth dynamics, can help explain their properties, and point to factors influencing their scaleability for device applications.

Here, we use the contrast from scanning electron microscope (SEM) images to unlock the metal intercalation positions as well as the EG thicknesses. We applied multiple correlative electron microscopy techniques for understanding the secondary electron (SE) emission that generates the contrast in SEM images. Our correlative electron microscopy includes surface chemical maps in plan view using auger electron spectroscopy (AES) and with Scanning-Transmission electron microscopy (STEM) imaging and electron energy-loss spectroscopy (EELS) obtained from multiple site-specific cross-sections (Figure 1). We also understand the origin of the SE emission related to the heterostructure's local work function by correlating both experimental measurements and theoretical calculations of the surface potential of these heterostructures. We also optimized the SEM imaging conditions – current, voltage, contrast/brightness, and the SE detector – to efficiently augment the differential SEM contrasts, thus providing a rapid characterization path using only the SEM to identify van der Waals heterostructure growth morphology variations.

Deformation behaviors of three-dimensional graphene honeycombs under uniaxial in-plane compression

Yiqing Chen, Fanchao Meng, Jun Song

McGill University

Abstract:

Using atomistic simulations and continuum modeling, the deformation behaviors of three-dimensional (3D) graphene honeycomb structures under uniaxial in-plane compression have been systematically investigated. It was found that the stress-strain responses of graphene honeycombs are dependent on the loading direction, prism size and lattice orientation, but little affected by the junction type. We identified two critical deformation events, i.e., elastic buckling and structural collapse, with the associated local and global structural changes clarified. In accordance with the continuum theory, analytical models accounting for the effect of lattice orientation and size-dependent yielding have been developed to quantitatively predict the threshold stresses for those critical deformation events. In addition, it has been demonstrated that the overall stress-strain curve of graphene honeycomb can also be reasonably well predicted via continuum modeling, albeit deviation at large strains due to the effect of junction on cell wall bending. The present study provides critical mechanistic understanding and predictive tools for optimizing and designing 3D graphene honeycombs in small-scale applications.

Defects and Quantum States based on Bi/Si(111) System

Longxing Chi, Chandra Veer Singh, Jun Nogami

University Of Toronto

Abstract:

Bi/Si(111)-√3×√3 surface reconstruction is a promising 2D system for spintronic fabrication and spin current control due to its extraordinary Rashba spin splitting.[1] Previous report has already covered the crystal and electronic structures of the system.[2] However, potential applications in quantum devices using its unique electronic states have rarely been mentioned. Here, we investigate the influence of defects and potential quantum applications of Bi/Si(111)-based 2D systems using scanning tunneling microscopy and density functional theory. First, connection between in-gap surface states and defects in the Bi/Si(111) system is interpreted. Analysis on the defect states perfectly convince the origin of in-gap surface states. Second, phase transition induced quantum dot states are observed on the Bi/Si(111) system, which can be easily achieved by thermal annealing. The quantum dot size can also be predicted by a kinetic fitting model during the transition. Finally, a 2√3×2√3 Pb superlattice can be achieved on the Bi/Si(111) surface, which exhibits strong Rashba splitting and can be used to fabricate quantum well devices.

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The formation and characterization of carbon-based 1D and 2D materials at the atomic scale

Maryam Ebrahimi

Lakehead University

Abstract:

The growing interest in 2D materials stems from their remarkable properties, such as high conductivity, heat transfer, mechanical, and chemical stability, and emerging quantum properties, arising from reduced dimensionality. At the intersection of chemistry, physics, and materials science, our research focuses on the controlled formation of candidate low-dimensional nanomaterials with engineered electronic properties and morphology. This is accomplished by surface-confined reactions to design low-dimensional nanomaterials whose properties can be tailored by their structural design, morphology, dimension, size, building blocks, and the chemical nature of the bonds which hold them together. We present the formation of single-layer 1D and 2D polymers, metal-organic networks, organometallic structures, and self-assembled molecular networks on noble metal single crystal surfaces. To identify their morphology, chemical nature, and electronic properties, we employ high-resolution scanning tunnelling microscopy and non-contact atomic force microscopy at the atomic scale, and X-ray photoelectron spectroscopy, complemented with density functional theory calculations. The chemical and thermal stability, structural design, charge mobility, and electronic properties of these low-dimensional nanomaterials make them promising candidates for various applications, ranging from nanoelectronics, gas storage, energy, and environmental applications.

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Friction of Ti3C2Tx MXenes: a combined experimental-theoretical investigation

Pedro Guerra Demingos, Peter Serles, Mahdi Hamidinejad, Li Ma , Nima Barri , Hayden Taylor, Chandra Veer Singh, Chul Park, Tobin Filleter

University of Toronto

Abstract:

The low friction of 2D materials allows their application as solid lubricants, with graphene and MoS2 being the most studied cases. However, MXenes, despite representing one of the emerging classes within this family of nanomaterials and having a wide range of promising applications, have only been scarcely studied for lubrication. In this work, the friction properties of Ti3C2Tx MXenes is investigated by Friction Force Microscopy (FFM) with a sharp diamond tipped cantilever. Furthermore, Density Functional Theory (DFT) is used to calculate the Potential Energy Surface (PES) of MXenes with different surface coverages, including both homogeneous and heterogeneous passivation schemes. While other 2D materials present layer dependent friction properties and thus require multilayer systems for lubrication, MXenes presented the same friction coefficient at mono, bi and trilayer, which makes them uniquely promising as solid state lubricants at monolyer thickness. DFT assigned this behavior to MXenes having higher binding energy and activation barrier for interlayer shear than graphene, causing its friction behavior to be controlled by the diamond-MXene interface. DFT also estimated that OH termination induces higher binding energy due to the formation of hydrogen bonds, which results in a more corrugated PES and higher friction. Therefore we propose annealing as a method for enhancing the lubricating properties of MXenes, as it favoured O and F terminations and caused a reduction of 16-57% in friction, in accordance with the 34% estimated by DFT with similar heterogeneous coverages. Overall, we demonstrated for the first time that the lubricating properties of MXenes are uniquely placed among 2D materials in terms of mechanisms and capabilities, with low friction at the monolayer scale which can be further reduced by annealing.

2D electrides: a different type of two-dimensional material for nanoelectronics

Jesse Maassen, Fouad Kaadou, Vahid Askarpour, Mohammad Rafiee Diznab, Erin Johnson

Dalhousie University

Abstract:

2D semiconductors offer a host of exceptional and tailorable electronic properties, however a major challenge for their widespread use in device applications is the difficulty in forming low-resistance metal contacts. Parasitic contact resistance can significantly hinder device performance by reducing current and switching speed, and increasing power consumption. Issues that impede ohmic contacts to 2D semiconductors include Fermi-level pinning and the presence of a tunneling barrier across the metal-semiconductor junction (originating from van der Waals interactions). Given the importance of this problem, achieving ultra-low contact resistance with 2D semiconductors has been the focus of much research.

A novel strategy that we are pursuing to achieve this goal uses a 2D electride as an interfacial layer between the metal and 2D semiconductor. Layered electrides are bulk ionic solids comprised of weakly-interacting atomic layers with the conducting electrons located in the interstitial regions between the atomic layers. Since the electrons are physically separated from the lattice, layered electrides display unusually low electron-phonon coupling, high conductivity and low work function. In this talk, we present our work using first-principles atomistic modeling to explore the properties of 2D electrides and their application in 2D semiconductor-metal contacts. Our analysis of a MoS2-Ca2N-Au heterojunction demonstrates that the 2D Ca2N electride donates nearly all of its surface charge leading to the metalization of the 2D MoS2 semiconductor and a barrier-free contact. The findings from this work suggest that the insertion of a 2D electride is a promising strategy towards achieving record low resistance, ohmic contacts in nanodevices.

Machine learning assisted quantification of relative thermodynamic stability and stiffness of 2D materials

Hema Rajesh Nadella, Sankha Mukherjee, Chandra Veer Singh

University of Toronto

Abstract:

Nano-scale thickness makes it challenging to experimentally evaluate the properties of 2D materials. Although high throughput databases are available, material models that capture the chemistry – structure – property relations of even the basic thermodynamic and mechanical properties of 2D materials are still at a nascent stage. To bridge this research gap, Gaussian process regression (GPR) machine learning (ML) models are developed to extract the chemistry – structure – property relations and predict 4 fundamental properties, per atom normalised ground state potential energy E_norm, heat of formation ΔH_form and in plane elastic constants C_11 and C_22 of a wide range of 2D materials. Uncertainty estimation, effortless hyper parameter tuning, easily generable features and magnetic state based material property prediction are the notable advantages of the current GPR ML models that makes them efficiently adaptable, easily trainable, highly transferable and completely reliable. Prediction errors in E_norm and ΔH_form values are as low as < 0.1 eV/atom. Average prediction errors in C_11 and C_22 values of experimentally synthesized 2D materials are as low as < 10%. Moreover, the stiffness characteristics of mechanically stiff MXenes are also properly captured by the current ML models. Hence, the GPR ML models developed in this study are suitable for a preliminary assessment of thermodynamics behind material formation and stiffness of 2D materials which is orders of magnitude faster than density functional theory (DFT) calculations or experiments. Also, the current ML models found few potential 2D materials with superior stiffness in other unseen databases during model training.

Oxidation-Controlled Nanoporous Graphene Oxide Membranes for Highly Selective Desalination

Claudio Adrian Ruiz Torres, Jay Werber

University of Toronto

Abstract:

Graphene and two-dimensional (2D) materials have been widely used for membrane fabrication for desalination, water/organic solvent treatments, gas separation, and energy devices. Among the various membrane structures based on 2D materials, multi-layered graphene oxide (GO) membranes have shown particularly promising performance in fluid separation processes, with selectivity achieved mainly through the size of interlayer spacing with a partial contribution of electrostatic interactions. However, in desalination, the swelling of GO laminates in water promotes the enlargement of interlayer spacing (d) to ~13.5 Å, restricting the ability to retain common salts. Several approaches have been suggested to suppress the interlayer spacing expansion, including physical confinement, crosslinking, or partial reduction, but stable and high ion rejection rate has yet to be realized. In this work, we prepare laminates of oxidation-controlled nanoporous graphene (OCNG) through graphite intercalation chemistry and vacuum filtration. The presence of nanopores was confirmed by electron microscopy and Raman spectroscopy. The controlled oxidation in the laminates shows a drastic reduction in channel swelling (8.9 Å after 24 h of immersion), reducing ion permeation 5-fold in comparison with fully oxidized graphene oxide. Using Forward Osmosis mode, our membrane demonstrated high retention of NaCl (>99%), including in harsh conditions, hypersaline feeds and 30 continuous days of operation. Our study demonstrates a significant advancement in the fabrication of nanoporous graphene-based materials and ion barriers for water desalination and electrochemical applications.

Defect engineering graphene for dynamic reliability

Boran Kumral

University of Toronto

Abstract:

The interface between 2D materials and stretchable substrates is a governing parameter in proposed 2D materials-based flexible devices. However, the same interface is dominated by van der Waals (vdW) forces and the mismatch in elastic constants between the contact materials leads to very low adhesion energy. Under cyclic loading, the low adhesion leads to decoupling, slippage, and extensive damage propagation in the 2D lattice. We reveal that through careful exposure to oxygen plasma, the interface can be functionalized to increase adhesion to drastically inhibit damage propagation under cyclic loading. This work offers insight into achieving dynamically reliable graphene-polymer contacts, which could facilitate the development of 2D materials-based flexible devices.

Posters:

Splendid Absorption-Dominant Electromagnetic Interference Shielding Effectiveness of Polyaniline Grafted Ti3C2Tx MXene/PVDF Composite

Saeed Habibpour, Chul B. Park, Aiping Yu

University of Waterloo

Abstract:

Nowadays, evolutions in wireless telecommunication industries, such as the emergence of complex 5G technology, occur together with massive development in portable electronics and wireless systems. This positive progress has come at the expense of significant electromagnetic interference (EMI) pollution, which requires the development of highly efficient shielding material with low EM reflection. Manipulation of MXene surface functional groups and, subsequently, incorporation in engineered polymer matrices provide mechanisms to improve electro-mechanical performance of conductive polymer composites (CPCs) and create a safe EM environment. Herein, Ti3C2Tx MXene nanoflakes were first synthesized and then, taking advantage of its abundant surface functional groups, polyaniline nanofibers were grafted on the MXene surface via oxidant-free oxidative polymerization at two different MXene to monomer ratios. The electrical conductivity, EMI shielding effectiveness (SE) and mechanical properties of poly (vinylidene fluoride) (PVDF)-based CPCs at different nanomaterial loadings were then thoroughly investigated. A very low percolation threshold of 1.8 vol% and outstanding electrical conductivity of 0.23 S/cm, 0.195 S/cm and 0.170 S/cm were obtained at 6.9 vol% loading for PVDF-MXene, PVDF-MX2AN1 and PVDF-MX1AN1, respectively. Compared to pristine MXene composite, surface modification significantly enhanced the absorption dominant EMI SE of the PVDF-MX2AN1 and PVDF-MX1AN1 composites by 19.6% and 32.7%, respectively. The remarkable EMI SE enhancement of the modified nanoflakes was attributed to (i) the intercalation of polyaniline nanofibers between MXene layers, (ii) a large amount of dipole and interfacial polarization dissipation by constructing capacitor-like structures between nanoflakes and polymer chains and (iii) augmented EMI attenuation via conducting polyaniline nanofibers.

Doped two-dimensional titanium disulphide (2D-TiS2) as potential anode material for lithium-ion batteries

Akhil Kunjikuttan Nair, Dr. Carlos Da Silva and Prof. Cristina Amon

University of Toronto

Abstract:

Energy storage technologies, such as batteries and supercapacitors, are being pushed toward greater power and energy density by the widespread usage of portable electronic devices and electric vehicles (EVs). Hence, the development of innovative materials is crucial for increasing the power, capacity, and energy density of batteries. The class of two-dimensional (2D) materials has demonstrated significant promise as active materials in lithium-ion batteries (LIBs), owing to their large specific surface area, which provide electrochemically active sites for ion storage and open 2D channels for rapid ion transit. Furthermore, tuning mechanisms such as doping were shown to enhance the electrochemical performance of 2D materials and enable their device applications. In this work, we explore the electrochemical properties of 2D TiS2 for its use in battery anode applications using density functional theory (DFT). The storage capacity of monolayer TiS2 was found to be 478.6 mAhg-1, which is 28.65% greater than that of graphite with the Li ion adsorption energy determined to be 2.03 eV/atom on the surface of monolayer TiS2. Furthermore, by substitutional doping of Co atoms on TiS2, the adsorption energy increased to 2.71 eV/atom, a 33.5% enhancement over the pristine condition, which makes Co-doped TiS2 to be potential contender for battery anode applications over traditional graphite and other 2D materials.

Electromagnetic interference shielding and EM wave attenuation with 2D MXene/polymer nanocomposites

Li Ma

University of Toronto

Abstract:

Recently, highly efficient Electromagnetic (EM) wave attenuation and Electromagnetic Interference (EMI) shielding materials are in great demand to address concerns associated with electromagnetic pollution. The rapid development of 5th-generation wireless systems contributes to intensified EM wave emissions to our environment. Moreover, EMI pollution can cause the malfunction of sensitive electronic components that may lead to system failures and potentially endanger human health. Conductive polymer composites (CPCs) incorporating highly conductive fillers, such as 2D MXene, have shown great promise as efficient EMI shielding materials.

However, despite the outstanding EMI Shielding Effectiveness (SE) of the CPCs reported in the literature, severe impedance mismatch at the solid/air interface results in the significant surface reflection of incident EM waves. In this context, achieving high EMI SE while minimizing reflection is significant in preventing secondary pollution.

As the continuation of our previous studies, a novel lightweight, layered foam/film PVDF nanocomposite with efficient EMI SE but ultralow reflection characteristics has been designed and developed. The unique layered foam/film structure was composed of PVDF/SiCnw@MXene composite foam as the absorption layer and highly conductive PVDF/MWCNT/GnPs composite film as the reflection layer. The heterostructure interfaces constructed between the 2D MXene and 1D SiCnw within the foam layer can effectively enhance the EM wave attenuation capability. Furthermore, the microcellular structure effectively tuned the impedance matching and prolonged the wave propagating path by internal scattering. Finally, the optimized layered foam/film PVDF nanocomposite exhibited an EMI SE of 32.6 dB and a low reflection bandwidth of 4 GHz (R<0.1) over the Ku-band at a thickness of 1.95 mm. A peak SER of 3.1×10^(-4) dB was obtained, corresponding to only 0.0022 % reflection efficiency.

Additive and advanced manufacturing of materials

Oral presentations:

Numerical Analysis of Diffusional Solidification Kinetics and Completion Time during Diffusion Brazing of Dissimilar Materials

Oluwadara Afolabi, Olanrewaju Ojo

University of Manitoba

Abstract:

Despite the attractive potential of diffusion brazing in joining dissimilar materials, the diffusional solidification kinetics during the diffusion brazing of dissimilar materials are barely studied and not well understood in the literature. In this work, a numerical model which, in contrast to existing models, integrates multi-dimensional migration of solid-liquid interface and occurrence of liquid-state diffusion (LSD) during diffusional solidification, is developed and used to study diffusional solidification kinetics and completion time during diffusion brazing of dissimilar materials. Variable spatial discretization technique based on the Murray-Landis Space Transformation and a unique adaptation of numerical winding in a hybrid implicit-explicit finite difference approach are used in the new model to ensure solute conservation and avoid the assumption of concentration-independent solid-state diffusivity. Notwithstanding two opposing factors – (i) loss of one substrate's contribution to diffusional solidification and (ii) extra liquid produced –, numerical analysis shows that diffusional solidification completion time can be shorter during diffusion brazing of dissimilar materials compared to similar materials. This is due to enhanced rates of diffusional solidification produced by LSD, which overcomes the two opposing factors. Nevertheless, a unique behavior is found for the first time by theoretical analysis in this work. It is found that it is possible for the completion time during dissimilar joining to be longer than when similar materials are diffusion brazed, despite an enhanced diffusional solidification rate enabled by LSD during dissimilar joining. This seeming anomaly which has been reported experimentally but not adequately explained in the literature, is found to be ascribable to a lower solid-state diffusivity and/or higher solidus concentration in the substrate melting than the one undergoing solidification during dissimilar diffusion brazing.

Assessing the Processability of CoCrFeMnNi fabricated with Selective Laser Melting.

Joseph Agyapong, Alexander Czekanski, Solomon Boakye-Yiadom

York University

Abstract:

Powder Bed Fusion (PBF) is an additive manufacturing process that uses powdered metallic materials to create intricately shaped objects. Recent technological improvements, particularly in-situ process monitoring, have resulted in the emergence of a new field of research devoted to the creation of alloys by and for PBF. As a result, such in-situ investigations can assist us in determining which challenges in the powder fusion process contribute to the part's final quality. This method is extremely effective for developing and screening novel alloys with a variety of compositions. High Entropy Alloys (HEAs) are composed of numerous elements with high concentrations of each. Thus, HEAs serve as competitive candidates for evaluating the feasibility of PBF alloy screening methodologies. This is because HEAs represent a potentially huge space in which candidate combinations must be screened. The purpose of this study is to select FeCoCrMnNi as a model HEA material for temperature profiles and on-line photography. The study will specifically monitor the behavior of multi-material printing using PBF methodologies, analyze the homogeneity of printed samples by altering the processing energy density, and characterize the material's mechanical and microstructural features. This enables us to comprehend and value PBF as a specially viable method for fabricating HEAs. The details will be discussed.

Auxetic Structures Produced of Aluminum Using a Combination of Stereolithography and Investment Casting

Nicholas Alfano, Abdallah Elsayed, Hari Simha

University of Guelph

Abstract:

Investment casting produces structurally complex metal parts with good surface finish, and attractive mechanical properties. Metal additive manufacturing using either powder bed fusion or direct energy deposition technology allow for significant design freedom, but the equipment is capital intensive. This study combines polymer additive manufacturing through the utilization of a stereolithography 3D printer and metal investment casting to produce complex geometry, lightweight structures for energy absorption in transportation applications. Investment cast 319 aluminum alloy as well as a pure aluminum, both with several investment-mold temperatures, melt-pouring temperatures, and vacuum levels were used to produce open celled, non-stochastic auxetic structures. The aluminum auxetic castings produced using higher vacuum levels of 100 kPa and lower investment mold temperatures of 600oC had fewer filling defects and were best able to replicate the stereolithography model while yielding the highest mechanical properties. The 319 alloy showed a rapid rise in load during compression testing to a peak of 16,653 N with a subsequent quick drop due to its lack of ductility while the pure Al sample maintained a load at 2900 N up to 60% strain. Typical casting defects included the presence of shrinkage pores and misruns at areas far away from the casting sprue. It is expected that optimization of the casting parameters can help eliminate these casting defects. The resulting aluminum auxetic structures and their production route offer an accessible method to produce high integrity, geometrically complex castings for transportation applications.

Experimental investigation of the multi-scale mechanics of advanced materials

Changhong Cao

McGill University

Abstract:

Continued advances in engineering technologies with increased complexity, enhanced performance and new capabilities, demand novel material systems with unprecedented properties as well as novel manufacturing approaches to accelerate the transfer of lab-scale inventions to the marketplace. Advanced materials, such as nanotubes and nanofilms, were demonstrated to be promising candidates for various applications including energy storage, electronics and transportation vehicles. Before advanced materials-based inventions can be widely applied to everyday life, their mechanical stability needs to be investigated, validated and engineered because it determines their long-term viability in all their applications. Also, by understanding the mechanical behaviors of advanced materials, novel material systems with tailored mechanical properties can be rationally designed for targeted applications. In this talk, I will use graphene oxide as a representative material to showcase the experimental explorations of its multiscale mechanical behaviors from sub-nanometer scale to microscale as well as mechanics-guided design of novel material structures for the assembly of electronics.

Enhanced tensile ductility of an additively manufactured AlSi10Mg alloy by reducing the density of melt pool boundaries

Haoxiu Chen, Sagar Patel, Mihaela Vlasea, Yu Zou

University of Toronto

Abstract:

AlSi10Mg components produced by laser powder bed fusion (LPBF) typically exhibit higher strength but lower ductility than those made by conventional casting. The effect of melt pool boundaries on the fracture behaviour of the LPBF-produced AlSi10Mg has not been systematically studied. Here we investigate the local strain evolution, microvoid growth, and crack formation in the melt pool boundary regions using in situ tensile testing and synchrotron-based X-ray microtomography. We show that decreasing area fractions of melt pool boundaries from 5.48% to 4.48% leads to an increase of tensile ductility from 7.2% to 9.8% in the LPBF AlSi10Mg samples. By controlling the density of melt pool boundaries in the LPBF process, we offer a new opportunity to fabricate AlSi10Mg products with an excellent combination of high strength and ductility.

Influence of Laser Parameter on the Tribological Behaviour of AlCoCrCuFeNi Laser-Deposited High Entropy Alloy

Modupeola Dada, Patricia Popoola, Ntombi Mathe

Tshwane University of Technology, Pretoria, South Africa

Abstract:

Wear is a destructive phenomenon and one of the principal causes of material failure in moving components during surface interaction while in service. High entropy alloy with its many properties is potential material for aero-engine applications. Investigation into the tribological behavior of AlCoCrCuFeNi HEAs is essential to reduce maintenance costs and prolong the service life of this advanced material for aerospace applications. However, most high entropy alloys are fabricated via arc melting, which has been reported to have defects attributed to slow solidification, consequently reducing the mechanical properties of the alloy. Therefore, there is a need for the use of advanced manufacturing techniques for fabricating these alloys. In this study, AlCoCrCuFeNi was fabricated via Laser Metal Deposition, the influence of the laser processing parameters, rapid solidification and the applied load on the tribological properties of the as-built alloys under dry conditions have been studied. The results showed that at a high laser power of 1600 W, a scan speed of 12 mm/s, and an energy density of 66.7 J/mm2, the lowest wear rates were observed. The average coefficient of friction at room temperature was 0.1 and 0.3 at a speed of 21 m/s. The dominant wear mechanism was abrasive wear as the wear rate and friction coefficient decreased with an increase in load from 10 N to 20 N. The scan speed had the most significant influence on the wear behavior of the as-built high entropy alloy attributed to the rapid rate of solidification which occurs at higher scan speeds.

Additive Manufacturing and localized material sourcing for sustainable manufacturing

Dr. Onyeka Franklin Ochonogor

Futuristic Engineering and Technology Group

Abstract:

Additive Manufacturing is becoming more interesting in this 4th industrial era as it has the potential to advance sustainable manufacturing. Project will address various Additive manufacturing challenges and improvement strategy as it relates to the development of new material for localized AM applications. Challenges in terms of material availability, digitalization and enabling production technologies provide new opportunities that have not been explored. It is about decentralizing manufacturing and making it autonomous near end user-driven activity.

The outcome of this project may form bases for new small and medium enterprise based on Additive manufacturing applications t o metal coatings which could be developed to support the local AM industry and generates much needed employment in South Africa.

High cost for materials is a major challenge affecting the adoption of Additive manufacturing in certain industries. Consumer demands for more customized products are on the rise, therefore more reliable means of sourcing materials has become inevitable. Identification and recycling of localized waste materials for AM feedstock is proposed to advance sustainable manufacturing. Various recycled materials will be biodegraded and combined in an attempt to form hybrid components. Biocompatibility and related properties will be investigated and evaluated. Components with high performance are expected to be developed, targeted at solving immediate community problems such as Low energy production (load shedding), high carbon emission of generating systems/cars and possibly find application in the aerospace, automotive industry, scaffolds for biomedical implant, sport equipments, jewellery product e.t.c.

New techniques and advanced engineering materials shall be developed, training of local students shall be carried out.

Microstructural, Mechanical, and fracture analysis of friction stir welded joints of high-temperature P22 steel and Al-Mg alloy

Dheerendra Dwivedi

Indian Institute of Technology Roorkee

Abstract:

Aluminum and steel dissimilar joints have a wide range of industrial applications, particularly in the automobile industry. Due to several challenges associated to their thermal and metallurgical properties mismatch, traditional fusion joining of Al-steel is often avoided. The melting and re solidification issues were eliminated using friction stir welding, a solid-state joining technique. A non-consumable WC tool is used to butt weld Al5052 and P22 steel plates in the current study. To determine the extent of metallurgical mixing, the joint is characterized using optical microscopy. Scanning electron microscope (SEM) and Energy dispersive x - ray spectroscopy (EDS) are used to quantitatively measure the intermetallic compound layer (IMC) that forms at the interface. Tensile and hardness studies are used to determine the mechanical properties of the weld joint. Steel fragments' involvement in joint morphology is briefly explored, and their impact on Al-steel joint fracture behavior is investigated. Further, it is concluded that an IMC layer formed in the FSW process is not detrimental to the joint's strength, whereas the steel fragments assisted the early fracture of the Al-steel joint.

Effects of Build Parameter Strategies on Surface Quality in 316L DMLS Prints

Lucas Gallant, Dr. Amy Hsiao, Dr. Grant McSorley

University of Prince Edward Island

Abstract:

Efficient printing of direct metal laser sintered (DMLS) parts is limited by poor surface quality, especially for overhanging geometries. Stair-stepping, balling, adhered powder material, and warping contribute to high roughness and form errors for these surfaces, and support structures are generally applied to inclines below 45°. Addressing as-built surface quality in the printing process through build parameter adjustments would reduce post-processing and support material. This work explores various build parameter conditions for potential surface improvements. Tests include comparing argon and nitrogen shielding gases, two powder particle size distributions, three adjusted exposure strategies using multiple contours, and a response surface DOE with laser power, scan speed, and hatch distance. Profilometry and 3D scanning techniques are used to evaluate surface quality for a range of geometries, with other properties of density, tensile strength, and residual stress also characterized. Results show improvements in upskin surface roughness for multiple contours and finer powder, increased tensile strength of nitrogen-printed samples, and over 25% improvement of downskin roughness from optimized exposure parameters, with relative density above 99%.

Propagation of cracks in amorphous materials: a molecular dynamics study using kinetic Activation-Relaxation technique

Renaud Girard, Ludvik Martinu, Normand Mousseau

University of Montreal

Abstract:

The use of amorphous materials in the form of thin films and coatings is widespread in high-tech components such as those used in optics and photonics. The performance of such films can deteriorate with time (aging) due to an interplay between the external solicitations (mechanical, thermal and environmental loads) as well as internal characteristics including the presence of defects, porosity, columnar structure and residual mechanical stress. Eventually, when the solicitations accumulate above a certain value, the films can fail due to cracking and crack propagation. While the propagation of cracks in crystalline materials is a process involving grain boundary, the crack propagation in amorphous materials follow no such logic since the regions where the bonds are weaker are not well defined (pores, inter-columnar structure etc.). The objective of this study is to develop a method to identify the mechanisms behind crack growth in amorphous materials, determine their resistance to crack formation for a specific material, and how cracks propagate through an interface of thin films on long time scales using the kinetic Activation-Relaxation technique (kART)[1]. Here we present preliminary results on a thin film of Stillinger-Weber amorphous silicon.

Microstructural Characterization of Wire Arc Additive Manufactured C250 Maraging Steel

Lulu Guo, L. Zhang, J. Andersson, O. Ojo

University of Manitoba

Abstract:

Multiple layers of C250 maraging steel were built into a single-wall structure with the use of wire arc additive manufacturing (WAAM) process. The solidification structure and phase characteristics of the as-fabricated C250 steel are studied by using optical microscopy, scanning electron microscopy, and transmission electron microscopy (TEM) techniques. The results reveal that lath martensite and austenite phases are formed in the wire arc additive manufactured C250 steel. Moreover, Laves phase Fe2Ti particles, which have not been previously reported in C250 maraging steel, are also observed in the wire arc additive manufactured C250 steel. Laves phase particles are known to be detrimental to mechanical properties and could also tie down important alloying elements that are required for forming strengthening precipitates. TEM analysis reveals the absence of required strengthening precipitates in the C250 steel after the WAAM process, which is in good agreement with hardness measurement results. The presence of the Laves phase and lack of strengthening precipitates in the wire arc additive manufactured C250 steel require sufficient consideration in the design of proper post-additive-manufacturing heat treatment for the steel.

3D printed spacers for in-situ membrane cleaning and chlorination

Abdullah Khalil, Farah Ejaz Ahmed, Raed Hashaikeh, Nidal Hilal

New York University

Abstract:

Membrane fouling, which causes constant decline in the output flux of permeate, is one of the most challenging issues in the membrane-based filtration processes. It requires process interruption for manual membrane cleaning using harsh chemicals to clear the membrane pores and restore the output flux. In this work, we demonstrate direct 3D printing of electrically conductive interdigitated spacer on polyethersulfone (PES) ultrafiltration (UF) membrane for in-situ membrane cleaning and chlorination via periodic electrolysis. The spacers were 3D printed on the membrane surface via material extrusion using a composite slurry of graphite, silver nanoparticles and PES. This composition allowed smooth 3D printing of electrically conductive spacers directly on to the membrane surface. Moreover, the spacers exhibited good mechanical flexibility and integrity with the PES-based UF membrane. The printed spacers promoted turbulence, thereby increasing the permeate flux in the presence of humic acid as a foulant. As the electric potential is applied across the two symmetric spacer segments in the presence of saline water as an electrolyte, bubbling at the cathodic segment due to the hydrogen evolution causes physical removal of the adhered foulant from the membrane surface leading to flux recovery. In parallel, chlorine evolves at the anodic segment which also aids in disinfecting the membrane surface as well as decomposing the organic foulants. Therefore, direct 3D printing of electrically conductive spacers on the membrane simultaneously offers four benefits: 1) spacer effect i.e. promoting turbulence and increasing the permeate flux in the presence of foulant, 2) in-situ membrane cleaning for flux restoration, 3) in-situ chlorination, and 4) a reduced build-envelope due to the integration of both anode and cathode with the membrane as spacer which eliminates the need for a separate spacer and the counter-electrode.

Offsize particle size utilization for laser powder bed fusion of Ti-6Al-4V powders: effect of powder properties on the performance of produced parts

Manvinder Lalh, Mahdi Habibnejad-Korayem

University of Toronto

Abstract:

Direct metal laser melting is an additive manufacturing process that utilizes a laser to fuse powders in a bed and typically utilizes fine powders with a narrow particle size distribution. Powder properties such as morphology, mean size and particle size distribution affect the flow properties of the powder, which in turn have strong effects on the performance of the final part. Previous work surrounding metal powders used in additive manufacturing focuses on the relationships between powder particle size distribution and flow properties. However, relationships between powder particle size distribution (PSD) and mean size to mechanical properties such as yield strength, tensile strength, dimensional accuracy, and surface roughness have not been explored. This work measured the flow properties of Ti-6Al-4V powders with varying size distributions and compared them to their mechanical performance and surface characteristics of laser powder bed fusion (LPBF) printed test coupons. Despite differences in powder size distribution mean size and flowability, the mechanical properties of each test coupon are comparable. The fracture surface and microstructure of each produced sample was nearly identical regardless of PSD. Results are promising in that they demonstrate that offsize PSD powders can generate coupons with comparable yield strength, tensile strength, hardness, and dimensional accuracy to the benchmark powder while also reducing explosivity. The main downside of utilizing offsize PSDs is that the surface roughness of the samples increase, though this increase is marginal when comparing to other manufacturing methods. Further work is required to fully understand the property interactions to fully define relationships between PSD and part properties

Structural Optimization for Fused Filament Fabrication Components using Stochastic Material Models

Gary Li, Craig Steeves

University of Toronto Institute for Aerospace Studies

Abstract:

The aim of this research is to develop an efficient and robust structural design method for Fused Filament Fabrication (FFF) manufactured components that accounts for the material variability inherent in this manufacturing process. FFF uses layerwise deposition of melted polymer filament and, as a consequence of the fabrication process, FFF components exhibit material property variations due to uneven filament heating, voids and defects induced during the manufacturing process. Not accounting for this could result in designs that significantly deteriorate in performance in practical applications.

Topology optimization (TO) is used to design structural components with complex shapes tailored for specific objectives, such as maximizing structural stiffness for a limited amount of material. TO designs can be efficiently manufactured using FFF, but unless the material model used for design accounts for the variability in material properties, the component may not perform as predicted. Here, the material model explicitly represents the property variations of FFF materials using a random field statistical surrogate, which is propagated into TO using uncertainty quantification (UQ) tools. The random matrix method (RMM) is the UQ method used to formulate a novel stochastic TO framework. RMM allows the design objective to have closed-form expressions, which is advantageous in improving the efficiency of gradient-based TO. Integration of a stochastic material model into the RMM TO framework results in an efficient and uncertainty-aware structural design tool for FFF components. Using benchmark problems, the performance of this tool is compared with established stochastic TO frameworks, such as the Monte Carlo method or stochastic collocation. This tool will help engineers generate robust designs that are less susceptible to variations in material properties, and that can, as a consequence, be made lighter and more efficient.

Effects of TiB2 in an Al-Cu-Sc Lattice Structures in the Hybrid Investment Casting Process

Yifan Li, Dr. Jose Marcelino, Dias Filho Aleeza Batool, Prof. Ahmed, Prof. Hani Henein

University of Alberta

Abstract:
The abstract needs approval from sponsors, it will be uploaded as soon as it is approved.

Enhanced tensile ductility of an additively manufactured near-α titanium alloy by microscale shear banding

Zhiying Liu, Daolun Chen, Yu Zou

University of Toronto

Abstract:

Laser-based directed energy deposition (LDED) enables rapid near-net-shape fabrication of large-scale titanium components for aerospace applications. However, the relatively poor tensile ductility of most as-deposited titanium alloys, particularly near-α alloys, hinders their wide usage for critical load-bearing structures. Here we report that a high density of microscale shear bands (MSBs) can be activated in an LDED-produced Ti-6Al-2Zr-Mo-V alloy with dispersed microscale α colonies to considerably enhance its tensile ductility. Using high-speed nanoindentation and in situ scanning electron microscopy tensile tests, we correlate the local micromechanical properties and global mechanical behaviour of such a LDED-produced titanium alloy: (i) The soft α colonies with a hardness of ~3.3 GPa produce slip bands (SLBs) with basal and prismatic <a>-slips; (ii) The surrounding hard α colonies or individual laths with a hardness of ~4.4 GPa are plastically deformed by activating MSBs, which are assisted by pyramidal <a>- and <c+a>-slips. Our results suggest that the nucleation of MSBs relies on the degree of local shear stress acting on the hard domains. The local shear stress is determined by the domain size, spatial orientation, and mechanical contrast with vicinal soft domains. The propagation of MSBs can be arrested by the boundaries between hard and soft domains, suppressing the evolution of MSBs into macroscale catastrophic shear bands and, therefore, enhancing tensile ductility. Our study demonstrates that activating the MSBs, by local microstructure and micromechanical design, provides a new opportunity to effectively enhance the ductility of LDED-produced titanium alloys and expedite the adoption of this additive manufacturing technology for critical structural applications.

Unit cell modelling of auxetic structure

Reem Roufail, Sydney Emma Pthier

University of Waterloo

Abstract:

Auxetic material structures exhibit a negative Poisson ratio. The structure expands in the axial and transverse directions under tensile loading and vice versa under compression loading. Many fabricated designs for auxetic materials exist such as re-entrant hexagonal, chiral, and arrowhead geometries. This paper studies the unit cell of the re-entrant hexagonal geometry to understand how changing the internal angle and fillet radius of the structure affects the Poisson's ratio. The material chosen for this study is acrylonitrile butadiene styrene (ABS) due to its availability and frequent use in additive manufacturing. The study was based on finite element analysis. It is observed that the direction of load applied to the unit cell affects the unit cell strain, Poisson's ratio, and maximum load capacity before failure responses. It is noticed that the re- entrant cell starts by showing a standard non-auxetic behavior until it reaches a specific axial strain value. A quadratic correlation is identified between axial and transverse strain. Designing an auxetic structure starts with understanding the behavior of a unit cell structure. The auxetic structure design is a complex process that requires a compromise between auxetic property to achieved and load capacity via avoiding stress concentration zones.

Compressive Behavior of As-built Laser Powder Bed Fusion AlSi10Mg Under Various Strain rates; Shear Band Formation

Adib Salandari Rabori, Vahid Fallah

Queen's University

Abstract:

A comprehensive study has been carried out delving into the strain rate dependency of compressive behavior of as-built Laser Powder Bed Fusion (LPBF) AlSi10Mg under constant strain rates as well as via strain rate change tests. Formation of shear bands in this alloy under compression is reported for the first time. It was found that the as-built printed AlSi10Mg is significantly strain rate sensitive in the range of 10-4 – 5 1/s strain rates (quasi-static to medium-dynamic) at the ambient temperature. A behavior that has not been reported for either cast counterparts or LPBF samples (either in the as-built or heat-treated states). In addition, the severity of shear band formation is found to be reliant on the imposed strain rate. These microstructural instabilities are shown to significantly influence strengthening and work hardening behavior. The shear band formation mechanisms and their interaction with other active plastic deformation mechanisms are thoroughly discussed.

Keywords: AlSi10Mg; LPBF; Compression; Shear Band; Strain Rate

Modelling of single pass wire and arc additive manufacturing

Anqi Shao, Jonas Valloton, Ahmed Qureshi, Hani Henein

University of Alberta

Abstract:

Wire and arc additive manufacturing (WAAM) is a type of direct energy deposition method and one of the additive manufacturing (AM) processes with the highest throughput. It is based on welding technology, using an electric arc as a heat source and a metallic wire as feedstock. Motion can be provided using a robotic arm or a gantry system. When melted, the feedstock material is deposited onto a substrate in the form of beads. A layer of metallic material is created as the beads coalesce. The process is then repeated layer by layer until the metal part is completed. In this work, single strands or stringers of ER70S-6 (UNS K11140) are deposited with the WAAM process. The strands are then modeled using the Additive Manufacturing module of Abaqus. The cooling rate and solidification time of the deposited layer thus obtained are modeled and compared to microstructural examination of the stringer sample. This approach is aimed to determine the initial solidification structure of any layer deposited during an AM build of a component.

Tool Failure by Aluminum galling on steel tools during punching of AA5754-O sheets

Shayan Shirzadian, Sukanta Bhowmick, Ahmet T. Alpas

University of Windsor

Abstract:

Tool wear and chipping are the main failure mechanisms that occur during machining and forming of ferrous alloys, while the failure of the tools used for forming of aluminum alloy sheets is triggered by galling. Galling occurs as a result of large-scale material transfer from the workpiece to the tool surfaces, shortening the tool life, increasing the energy expenditure during each cycle of a forming or shaping process, and lowering the surface quality of the sheets. To increase the cost-effectiveness of aluminum forming operations and enhance the product's surface quality, the study of galling is highly important. However, there is a lack of a reliable galling measurement technique to quantify the amount of galling. A new galling volume measurement technique is developed in this study using white light interferometry. Shear-punch tests on AA5754-O sheets allowed investigation of the progression of galling on uncoated and diamond-like carbon (DLC)-coated steel tools. Tests were performed under two different lubrication methods. Unlubricated (dry) punching tests were also performed. In punching with DLC-coated tools, the coating was detached from the punch surface after 20 strokes of dry punching and 30 strokes of punching if only the sheet surface was lubricated, whereas a near-zero galling volume was recorded after 500 strokes if the tool was lubricated as well as the sheet surface.

Laser Powder Bed fusion of Aluminum-Copper alloy

Satish Kumar Tumulu, Mathieu Brochu

McGill University

Abstract:

Laser Power Bed Fusion (LPBF) process, one of the major processes in additive manufacturing (AM), has been successfully utilized to fabricate metal components. The bulk of the literature and knowledge on AM of Al alloys focuses on the Al-Si-Mg system, which has moderate strength, therefore not suitable for high strength applications. Thus, there is a demand to find a compatible alternative alloy to AM with higher strength for wider application. Aluminum Copper (Al-Cu) alloys are high strength Al alloys typically used in the aerospace industry. Most of the 2XXX alloys have not been extensively explored for LPBF process due to their inherent solidification behavior, prone to cracking. Few approaches emerging for new alloy compositions is now changing this reality. In this seminar, we will present a complete LPBF process optimization study for Al-Cu-Ti alloy. High-density and defect-free components were successfully produced. To further increase the strength by precipitation strengthening, the LPBF parts were subjected to a heat treatment involving solutionising, followed by ageing. The microstructure obtained was analyzed in as built and heat-treated conditions to understand the microstructural development. The mechanical properties were assessed by microhardness, tensile and impact strength at room temperature for both conditions. Fracture surfaces of the tested samples were analyzed to understand the deformation behavior.

Effect of post-printing solution-aging heat treatment on the microstructure and corrosion properties of a wire arc additive manufactured PH 13-8Mo martensitic stainless steel

Alireza Vahedi Nemani, Mahya Ghaffari, Salar Salahi, Ali Nasiri

Dalhousie University

Abstract:

Over the past decade, wire arc additive manufacturing has become a promising alternative to conventional manufacturing methods due to its great potentials for fabrication of medium to large size components with high deposition rate, low raw material consumption, and flexibility in design. The implementation of WAAM for production of ferrous parts has been widely investigated. Regardless of the nature of any fusion-based metal AM process, the majority of AM fabricated ferrous alloys are not intended for service in as-printed condition, and they require an appropriate post-printing heat treatment process to deliver the desired microstructure and ultimately performance. In this study, the effect of post-printing solution and aging treatment on the secondary phase(s) formation and the resultant corrosion performance of an additively manufactured precipitation hardening martensitic stainless steel (PH 13-8Mo) were investigated. Multi-scale microstructural characterizations were performed using scanning electron microscope equipped with energy-dispersive X-ray spectroscopy, scanning transmission electron microscope, and X-ray diffraction technique. Electrochemical response of the as-printed and heat-treated samples were also measured using open circuit potential, potentiodynamic polarization, electrochemical impedance spectroscopy, and Mott-Schottky analyses. Microstructural characterizations and corrosion measurements revealed that solution treatment followed by aging at 400 and 500 °C significantly improved the corrosion resistance of the material due to the removal of Cr-enriched δ-ferrite phases from the as-printed microstructure, which trigger the sensitization phenomena in Cr-depleted region at the boundaries of δ-ferrite and matrix. However, aging at a high temperature (600 °C) resulted in the formation of Cr-enriched M23C6 carbides that created micro-galvanic coupling sites throughout the microstructure, adversely affecting the corrosion performance of the alloy.

Fabrication and Characterization of Dense Ceramic Coatings by Aerosol Deposition

Zhenying Yang

University of Toronto

Abstract:

Advanced ceramic coatings are attractive in many industries, ranging from microelectronics to aerospace. Fabricating dense ceramic coatings using established techniques is challenging due to the brittleness and high melting temperature of ceramics. Aerosol deposition (AD) is a solid-state coating process capable of producing dense nanocrystalline ceramic films. AD has attracted attention in the ceramic coating field due to its unique features, including the room temperature nature, high film density with crack-free structure, controllable coating thickness, relatively high deposition rate, good mechanical properties, and a wide choice of substrates. However, as a novel technique, the deposition mechanism has not been fully understood yet. This study aims to analyze the adhesion mechanism of AD, focusing on the effect of powder size and substrate properties on the first layer formation, also called the anchoring layer. A deposition system has been designed and assembled. Raw alumina (Al2O3) powders were pre-treated to obtain different particle sizes and size distributions. To illustrate the effect of substrate roughness and hardness, stainless steel, alumina, and glass plates were used.

Study on the removal of inclusions in liquid steel by the Nitrogen Elevating and Reducing Method

Shuo Zhang

University of Toronto

Abstract:

In order to explore a new process to improve the steel cleanliness by reducing the number of inclusions, Dongbei Special Steel Group Co., Ltd and University of Science and Technology Beijing carried out a set of industrial tests. The method, referred to as Nitrogen Elevating and Reducing Method (NERM) involves first nitrogenizing molten steel that elevates the nitrogen content and second applying vacuum to steel so that nitrogen bubbles form and aid in flotation of the inclusions to the surface. The removal efficiencies of the new and the conventional routes are presented and compared in this talk. The results show that NERM reduces the oxygen content representing the level of inclusion quantity from 8 ppm (parts per million) to 6.5 ppm in steel product. Besides, the new method shows better removal of inclusions, and the number of inclusions decreased by 70% compared to the conventional method. Only the inclusions larger than 10 μm in diameter can be removed by the conventional process, and the inclusion less than 5 μm can be further removed by the NERM. The new method is particularly effective on the non-wetting inclusions. The wetting inclusions are also removed, at nearly half the rate of the non-wetting inclusions.

Bonding mechanism in cold spray process: recent advances from a unit process

Ahmed A. Tiamiyu and Moses A. Adaan-Nyiak

Department of Mechanical and Manufacturing Engineering, University of Calgary, 2500 University Drive NW, Calgary, Alberta T2N 1N4, Canada.

Abstract:

Cold spray (CS) processing is a solid-state deposition process that involves the launch of micro-particles to sufficiently high velocities; these particles adhere to a substrate and previously deposited particles to form coatings/parts. Despite the advancements in applications of CS in the past decades, complexities from particle-particle/carrier gas interactions obscure assessment of particle bonding mechanisms. Hence, there are debates on which mechanism dominates the formation of bonds. This talk evaluates recent findings from single-particle impact approaches that circumvent these complexities and further provide new insights on bonding mechanisms. Although there is a unified condition for the onset of bonding—a pristine metal surface in contact at sufficient impact velocity, no singular existing theory explains bonding mechanism; the dominant mechanism is rather a function of the prevailing barriers unique to each impact scenarios.

Posters:

Aramid fabric-reinforced composites by electrospun P(An-co-GMA) nanofibrous interlayers

Farzin Asghari Arpatappeh, Cem Ünsal, Kaan Bilge, Farzin Javanshour, Sıla Güngör, Melih Papila

Sabanci University

Abstract:

This study reports the effect of electrospinning nanofiber interlayers of epoxy-compatible poly[acrylonitrile-co-(glycidyl methacrylate)], hereafter P(An-co-GMA), in the tensile properties of plain-weave aramid fabric-reinforced composites. Laminates of composites were interleaved by nanofiber mats of commercially available polyacrylonitrile and the copolymerized acrylonitrile with glycidyl methacrylate; a molecule containing an epoxide. This ring was supposed to break by the heat provided in the composite processing and make bonds to the same broken groups on the epoxy matrix. Free-radical polymerization was run in solution environment and the success of the polymerization was verified with FT-IR. Nanofibers mats were collected electrospinning of both PAN and P(An-co-GMA) and analyzed morphologically using FE-SEM. Laminates were prepared using vacuum bag-assisted hot-press molding and cut into desired geometry using a waterjet. The samples were tested according to the standard tensile tests. The results revealed that the interlayers of P(An-co-GMA) in epoxy-matrix increased the tensile modulus by 34%, the strength by 8%, and reduced the ductility by 2.5% when compared to virgin laminates. Polyacrylonitrile also improved the mechanical properties; increased the tensile modulus by 26%, reduced the strength by 13%, and reduced the ductility by 2.4%. When nanofibers interlayers of epoxy-compatible polymer laminated with phenolic matrix, the reinforcement mechanism changed from the improvement in the tensile modulus to an improvement in the tensile strength by 18%. In conclusion, epoxy compatible polymers showed promising results in improving the mechanical properties of composites both with their morphological advantages, and covalent bonding they created with the epoxy matrix. The approach can be applied for tailoring the properties of aramid fiber-reinforced composites in automotive and aerospace structures.

Weld cladding of Ni-based WC metal matrix composite overlays by CMT and standard GMAW processes

Mohammad Reza Karimi, Sheng-Hui Wang, Jasmin Jelovica

University of British Columbia

Abstract:

During weld cladding of Ni-based tungsten carbide metal matrix composite (Ni-WC MMC) overlays, the excessive dissolution of WC leads to brittle secondary carbide phase formation. The wear behavior of these overlays lies mainly in the existence of the retained hard WC particles. Dissolution of these particles during deposition adversely affects the wear-resistance of the overlay. The degree of WC dissolution is inversely proportional to the level of heat input.

In this research, standard gas metal arc welding (GMAW) and Cold Metal Transfer (CMT) processes are used to deposit overlays by employing tubular NiCrBSi WC wires on A36 steel substrate. Taguchi design of experiments L16 is used to investigate the effect of wire feed speed (WFS), travel speed, and shielding gas of these processes on volume fraction of WC, carbide transfer efficiency, deposition rate, hardness, dilution, and weld bead shape of resultant overlays. Results show that WFS is one of the most significant factors governing weld bead characteristics of the deposited overlays. For the volume fraction of WC, travel speed was found to be the most influential factor. In addition, CMT process is less sensitive to welding parameters than standard GMAW. CMT can also eliminate excessive dissolution of WC during the weld cladding process.

High Strain Rate Full-field Strain Evolution and Post Impact Hardness of Additively Manufactured Ti6Al4V-ELI

Diego Mateos, Ali Eliasu, Solomon Boakye-Yiadom

York University

Abstract:

The direct impact Hopkinson pressure bar (DIHB) is used in this research to study the mechanical behavior and formation of adiabatic shear bands during dynamic compression in Grade 23 Ti6Al4V-ELI processed by direct metal laser sintering (DMLS). Tests are conducted at strain rates of 2500 s-1, 3760 s-1, and 5300 s-1. Digital Image Correlation (2D-DIC) and optical microscopy techniques are employed on axisymmetric compression specimens to probe inhomogeneous surface strain distributions and adiabatic shear bands (ASBs), respectively. Additionally, pre and post impact Vickers microhardness tests are conducted with specific emphasis on the post-impact ASB regions. It is found that DIC can enable a data-informative representation of the time and position dependent evolution of deformation and strain throughout the specimen surface. Deformation fields in the axial direction show the effect of using a direct projectile, resulting in the propagation of the stress wave throughout the specimen. Deformation fields in the transverse direction show the evolution of the maximum shear stress plane throughout loading. It is observed that strain localization sites on the surface can be associated with potential fracture initiation sites and that the axial and maximum shear strains have similar surface distributions. Furthermore, it is demonstrated that potential fracture initiation sites can be quantified and the fracture direction can be predicted at an instant before failure. Lastly, it is found that the Vickers microhardness at the center of the ASB region is higher than the surrounding matrix and the pre-impact hardness for all strain rates.

Deformation Mechanism and Microstructure Evolution of Beta-C (Ti-3Al-8V-6Cr-4Mo-4Zr) Titanium during Diametrical Compression Test

Javier Miranda, Mike Bruhis, Hatem S. Zurob, and André B. Phillion

McMaster University

Abstract:

The room-temperature mechanical behavior of a beta titanium alloy known as Beta-C (Ti-3Al-8V-6Cr-4Mo-4Zr) has been studied using diametral compression testing (DCT). A circular disc was chosen as the sample geometry due to its geometric similarity to the wire flat rolling process that is used to fabricate the wire feedstock for additive manufacturing applications. Local strain maps were acquired via digital image correlation using an ARAMIS system. The change in microstructure as a result of DCT was studied using optical microscopy, scanning electron microscopy and EBSD. Analysis of the local strain maps revealed that the plastic deformation produces two diagonally oriented shear bands. Analysis of the microstructure revealed that twining, stress-induced α phase transformation and dislocation slip are the main deformation mechanisms. The acquired equivalent stress-strain curves show good agreement when compared against standard curves obtained via tensile testing. Overall, it is shown that the DCT technique is efficient in determining the stress and strain limits for flat wire/rod rolling processes.

Investigating the Evolution of Damage in Additively Manufactured AlSi10Mg

Youssef Salib, Darren Feenstra, David Wilkinson, Hatem Zurob

McMaster University

Abstract:

Additive manufacturing (AM) has gained a lot of popularity for its ability to produce unique parts of geometric complexity. This enables products to have complex geometries that are not otherwise able to be produced through traditional manufacturing methods, and it enables a high potential to make a component more lightweight. This is especially desirable for the space industry because of the high cost per weight of launching materials into orbit. Since AM has the ability to produce parts of high strength due to the rapid cooling rates associated with the process, the ductility will naturally suffer as a consequence. The material of interest is a popular aluminum alloy (AlSi10Mg) that contains 10% silicon and is widely used in the space industry for its good mechanical properties and light weight. This alloy will be studied to observe the impact of applying heat treatments on the damage evolution and mechanical properties of AlSi10Mg produced through additive manufacturing. Techniques such as in-situ tensile testing via x-ray computed tomography and in-situ tensile testing via SEM coupled with micro-digital image correlation (μ-DIC) will help connect microstructural features to areas of high strain localization and void growth, such that a process-structure-property relationship can be established.

Neutral pH polymer electrolytes for inkjet-printed electrolyte-gated transistors

Guan Ying (Jane) Wang

University of Toronto and National Research Council Canada

Abstract:

Electrolyte-gated field effect transistors (EGFETs) are one of the key components for printable, low-cost, low-power, portable, and flexible electronics such as wearable sensors. The evolution of these technologies would depend greatly on the development of inexpensive silver electrodes to replace expensive and process-intensive gold electrode contacts. We have evaluated the electrochemical stability, charge transport characteristics, and in-device performance of several proton- and neutral pH-ion conducting polymer electrolytes in EGFETs with the intention of improving electrolyte-electrode stability with silver electrodes. Our investigation revealed that electrolytes containing lithium nitrate (LiNO3) salt in a polyvinyl alcohol (PVA) matrix, a promising solid electrolyte for supercapacitors, can be adapted to EGFETs. LiNO3/PVA provides a high ionic conductivity and specific capacitance which are necessary for efficient electric double layer gating in sub-1V EGFETs. Using a blend of additive manufacturing techniques including inkjet and screen printing, we have fabricated EGFETs using LiNO3/PVA on silver and gold electrodes. In the presentation we will further expand on the techniques used as well as the characterization, evaluation, and optimization of these devices.

Advanced Materials Characterization (supported by Canadian light source (CLS))

Oral presentations:

Development of a Low-Cost Method for Screening Hypersonic Materials

Ben Antaya, Ali Merati

National Research Council, Aerospace Research Centre

Abstract:

Phase Differentiation of Zirconia Polymorphs in Low-Voltage Scanning Electron Microscopy

Farzin Asghari Arpatappeh, Cleva Ow-Yang, Sorour Semsari Parapari, Gülcan Çorapçıoğlu, Mehmet Ali Gülgün, Melih Papila

Univerisity of Toronto

Abstract:

The challenge is to differentiate polymorphs in SEM images, which is not possible in conventional SEMs since polymorphs have no atomic number difference, hence they do not create any contrast. However, they do have different secondary electron (SE) yields. This difference was used before to create contrast between various semiconductors, Cr-Mo steels with different precipitates, fungi, and ceramic composites. We demonstrated this new approach on tetragonal zirconia (t-phase) and monoclinic zirconia (m-phase). T-phase was partially stabilized tetragonal ZrO2 doped with 3 mol% Y (TOSOH). M-phase was synthesized from zirconyl chloride octahydrate (Fluka) by calcination at 1000 °C for 1 hour. The polymorphs were imaged in an FE-SEM (Zeiss Leo Supra 35 VP) with an accelerating voltage tunable between 150 V and 30 kV, with a step resolution of 10 V while collecting the signals with an in-lens detector. Micrographs of the SE signal of m-phase and t-phase was captured on an In-lens detector in an accelerating voltage range of 0.4 - 1 kV. This showed that there is a significant contrast between the phases so that m-phase always appears brighter than t-phase. In addition, this difference increases as the acceleration voltage decreases. Quantitative analysis using a Python computer code revealed that when the acceleration voltage is as low as 0.4 kV, the contrast between the phases surmounts 70%. Theoretical approach showed that the contrast comes from the difference in the electron affinity of the phases, which is higher for t-phase. Therefore, it has a lower SE yield, and appear darker in this method. The formulation also justifies the rise of the contrast, which happens when the acceleration voltage is reduced. This method appears to be a promising and feasible method for the differentiation of polymorphs that would not be distinguishable in an SEM unless using complex equipment. This method can be further improved to distinguish even smaller grains of polymorphs.

High-throughput Characterization of High-entropy Alloys Based on Synchrotron Diffraction and Machine Learning

Changjun Cheng, Renfei Feng

AGH University of Science and Technology

Abstract:

High-entropy alloys (HEAs) are novel multiple component materials, exhibiting promising mechanical properties at a wide temperature regime. For such materials, slight composition variance is usually accompanied by structure transition, which will subsequently affect the properties significantly. Some promising compositions are generally located at a narrow composition regime. Traditional methods can only fabricate materials with a single or just a few compositions, which drastically reduces the efficiency of subsequent testing, characterization, and further composition modification. In this work, by using the magnetron co-sputtering technique, we fabricate nanoscale HEA thin films with gradient compositions on Silicon wafers. Based on synchrotron X-ray diffraction and fluorescence mapping, we can obtain the structural and compositional distribution on the sample. However, due to a large amount of data and a high degree of composition freedom, it is hard to establish the relationship between composition and structure. In response, we propose the strategy using the machine learning method for high-throughput computation. Compared with unsupervised machine learning methods, the supervised ones can extrapolate the relationship with high accuracy. The logistic regression shows a similar performance to the neural network method, while it exhibits better interpretability and higher iteration efficiency.

The effect of corrosion on thermomechanical behaviour of alumina-spinel refractories

Sina Darban, Camille Reynaert, Ryszard Prorok, Jean Jillibert, Thomas Sayet, Eric Blond, Jacek Szczerba

Canadian Light Source

Abstract:

Refractory materials are ceramic materials that are used in the steel industry. Since refractories in steel ladles are in touch with molten slag and steel at high temperatures; they are exposed to high temperature corrosion during their working time and corrosion may affect the thermomechanical properties of refractories. In this study, the effect of corrosive medium (industrial slag) on thermomechanical properties of alumina-spinel refractories which are used in sidewalls and bottom of steel ladles investigated. For this means the impregnated alumina-spinel samples were prepared in laboratory condition and thermomechanical behavior of samples investigated by aid of Brazilian test coupled with digital image correlation (DIC) at 1200 °C. The phase composition and microstructure analysis were explored by x-ray diffraction method (XRD) and scanning electron microscope coupled with energy dispersive spectroscopy (SEM/EDS).

Applications of Hard X-ray microTomography for Materials Characterization at Canadian Light Source

Sergey Gasilov, Toby Bond, Andre Phillion

Canadian Light Source

Abstract:

X-ray computed tomography (CT) has become a widely used tool for 3D non-destructive imaging of materials. Laboratory CT systems can be used to image the microstructure of materials down to the micron scale. High-resolution scans are very slow however, often requiring a sample to be static for many hours.

The biomedical imaging beamline of Canadian Light Source produces 6 orders of magnitude more photons than a laboratory source in a collimated beam with very small divergence. This allows for much faster scan times, especially at micron-scale resolution, where scans can be completed in minutes or even seconds that would otherwise take hours on a lab scanner. This makes such beamlines very well suited to in-situ and time-resolved experiments that can capture structural changes due to applied mechanical, chemical, or thermal stress. Synchrotron CT also provides greatly improved contrast that can resolve differences between materials of similar density and composition (such as alloys or carbon fibers in resin) that cannot be resolved with laboratory systems.

This talk will provide an overview of synchrotron CT capabilities at the Canadian Light Source with a focus on applications in materials science. This includes examples from metallurgy, composites, battery materials, additive manufacturing, and other areas of active research. Highlights of ongoing and future technique development, such as in-situ tensile/compressive loading, in-operando scans, and a high-brilliance/high-energy imaging endstation will also be discussed.

Advanced Synchrotron Techniques for Materials Research

Feizhou He

Canadian Light Source

Abstract:

Synchrotron light source is a versatile and powerful tool for materials research. It is used to characterize a wide variety of materials, including engineering materials, catalyst, biological materials, and novel electronic materials.

This talk will provide an overview of the research capabilities at the Canadian Light Source, the national synchrotron facility of Canada, with a few research highlights such as non-destructive element-specific imaging, characterization of battery materials in action, and in-situ measurement of catalysts. These advanced imaging, spectroscopic and diffraction techniques are either impossible or very difficult without a synchrotron source. The researches enabled by synchrotrons are constantly pushing boundaries of materials science and engineering.

On the effects of microstructure on the development of 3D stress-fields near notches: measurement and modeling

Karim Louca, Hamidreza Abdolvand

National Research Council, Aerospace Research Centre

Abstract:

Understanding the impacts of cracks and notches on material behaviour in ductile alloys is crucial for developing macro- and microscale predictive models. The impact of microstructure near flawed geometries can be significant to the material's fatigue behaviour, specially in hexagonal close-packed (HCP) crystals with a high degree of elastic and plastic anisotropy. In this study, synchrotron three-dimensional X-ray diffraction (3D-XRD) is employed to investigate the effects of different notches on the grain-resolved tensorial stresses near the notch tips in pure zirconium specimens. The "as-measured" microstructures and notch geometries are subsequently imported into a crystal plasticity finite element (CPFE) model to simulate the evolution of stress, strain, and rotation fields. Stress distributions across the notches are further investigated for different paths to deconvolute the contribution of textures and microstructures to the development of stress concentration sites. Results show that load sharing between different grain orientations contributes significantly to the stress development in the vicinity of notches. As a result, grains with similar orientations undergo different plastic strain rates, depending on their positions with respect to the notch as well as their local grain neighbourhoods. It is shown that this load sharing mechanism strongly depends on the overall texture of the specimen and the notch geometry.

Hard x-ray diffraction and scattering beamlines for materials science at the Canadian Light Source

Beatriz Moreno, Adam Leontowich, Narayan Appathurai, Al Rahemtulla, Graham King, Chang-Yong Kim, Stefan Kycia

Canadian Light Source

Abstract:

The Brockhouse sector at the Canadian Light Source includes three hard x-ray beamlines recently built. These beamlines are dedicated to diffraction and scattering experiments for materials science. In this presentation, we will describe the new capabilities at these beamlines, enabling advanced materials characterization and cutting-edge science in Canada and abroad.

An in-vacuum wiggler and undulator provide bright beams to the beamlines resulting in competitive flux. Several specialized end-stations allow high-resolution powder x-ray diffraction, small angle x-ray diffraction (SAXS), wide angle x-ray diffraction (WAXS), pair distribution function (PDF), single crystal diffraction, reciprocal space maps (RSM), small angle x-ray reflectivity, anomalous / magnetic x-ray diffraction. Various sample environments are available for in-situ experiments as a function of temperature, pressure, gas atmosphere (static or flowing), vacuum, in-situ catalysis and battery cycling experiments. We have different detectors available --point, linear and area detectors--, allowing fast data collection and high-resolution time-resolved measurements.

Our capabilities find many applications in different materials research areas, including batteries, catalysis, cement, microelectronics, optoelectronics / perovskites, environmental and mineralogy research.

Our beamlines are now fully operational and open to users through our peer reviewed proposal system at the Canadian Light Source, www.lightsource.ca

The Development and Applications of Serial Electron Diffraction

Ehsan Nikbin, Daniel Zeitler, Asma Sarguroh, Robert A. McLeod, R. J. Dwayne Miller, Jane Y. Howe

University of Toronto

Abstract:

In scanning transmission electron microscopy (STEM), the image is formed by scanning a focused electron probe over the sample and collecting the transmitted electrons. Recent developments in software and hardware of electron microscopes enable collecting the diffraction pattern of the transmitted electrons for each scan point known as four-dimensional STEM (4D-STEM). The diffraction data can also be collected sequentially from selected points of the sample which is called serial electron diffraction (SerialED). SerialED/4D-STEM has been developed on a Hitachi HF-3300 transmission electron microscope (TEM)/STEM using the DigitalMicrograph scripting, and on a Hitachi HT-7700 TEM/STEM using the Azorus package developed by Hitachi High-Tech Canada.

In this work, SerialED/4D-STEM has been used for automated electron diffraction acquisition, recording the diffraction of beam-sensitive block copolymer micelles, crystal orientation mapping of a NiCo sample, and structure determination of nanocrystals. Normal diffraction acquisition involves finding a region of interest of the sample in the TEM imaging mode, and then switching to the diffraction mode to record the diffraction pattern. However, in SerialED, the crystals are selected from a low-dose STEM image of the sample, and the program collects the sequential diffraction data automatically for all chosen crystals. The effect of beam damage on the sample is also minimized, which makes it a suitable approach for diffraction acquisition of beam-sensitive materials. Grain orientation mapping of thin film materials can also be obtained by analysing the diffraction of each data point and finding the zone axis of the patterns. Finally, SerialED can be used as an alternative method to x-ray crystallography for structure determination of nanocrystals by collecting and analysing the diffraction data of randomly oriented crystals of the sample.

Real-time Analysis of Oxygen Vacancy of Indium Oxide via Environmental Transmission Electron Microscopy

Chenyue Qiu, Mengsha Li, Stas Dogel, Hooman Hosseinkhannazer, Lu Wang, Doug Perovic and Jane Howe

University of Toronto

Abstract:

Owing to the wide bandgap and limited number of oxygen vacancies of stoichiometric indium oxide, the utilization of solar energy is significantly hindered and limits its further development in the field of photothermal catalysis. Recently, it is found that the non-stoichiometric black indium oxide exhibited three orders of magnitude higher photothermal catalytic performance towards reverse water gas shift reaction than the stoichiometric indium oxide with 100% CO selectivity. The oxygen vacancies act as active sites and responsible for the remarkable photothermal activity. Furthermore, it would be of great scientific interest and technological important if a nanosized catalyst could be expanded at high temperatures and induce the formation of oxygen vacancies. To understand the relationship between microstructure and catalytic performance, we performed in situ heating scanning/transmission electron microscopy (S/TEM). The operation temperature ranges from room temperature to 450 ℃. The surface and center of the same nanoparticle were analyzed. At room temperature, the In2O3 NPs have a standard d-spacing of (222) plane at both surface and center regions. Intriguingly, at 450 ℃, the d-spacing of the surface region expands to 3.03 Å whereas that of the center region remains 2.91 Å. The electron energy loss spectroscopy (EELS) was performed to further detect the cause of d-spacing expansion from an oxygen concentration perspective. The EEL spectra demonstrate O-K edges for surface and center regions are located at the same energy loss positions at room temperature. In contrast, at 450 ℃, the surface and center O-K edge shifts to a lower energy loss position indicating the formation of oxygen vacancy and the larger shift of O-K edge indicates a higher oxygen vacancy concentration. Therefore, it is believed that oxygen vacancies are more favorably generated at particle surface acting as the primary factor to d-spacing expansion and the higher CO production rate.

Experimental Investigation on Surface Integrity of Commercially-Pure Titanium using Ultrasonic Pulsed Water Jet Peening

Paria Siahpour, Mark Amegadzie, Andrew Tieu, Mohan M. Vijay, Bryce Christensen, Ian W. Donaldson, Kevin Plucknett

Dalhousie University

Abstract:

'Water jetting' is a mechanical technique that has been mainly employed for surface cleaning, machining, and cutting of virtually all engineering products. Water jet peening (WJP) has been developed as a new cold-working surface strengthening process in many industrial sectors, from aerospace to automotive and medical industries. In comparison to the other conventional peening methods, including shot peening and laser shock peening, WJP is capable of producing smooth surface textures, high compressive residual stresses, resistance to corrosion, and improved fatigue strength. In this method, however, an appropriate selection of processing parameters such as jet pressure, standoff distance, traverse rate and exposure time, is considered challenging to obtain the optimum surface condition. In the present study, commercially pure titanium (CP-Ti) was subjected to a novel ultrasonic pulsed waterjet (UPWJ) peening approach, using a range of parameters to characterize and check the viability of UPWJ peening so that surface treatment can be achieved without causing any detrimental damage. The pulsating water jet was altered by varying the traverse speed within the range of 200 to 1000 mm/s, at stand-off-distances of 25.4 to 44.4 mm, using a water jet pressure of 69 MPa. Here, the impact of UPWJ on the microstructure, surface integrity, and topography/roughness of the treated surface was analyzed using confocal laser scanning microscopy, scanning electron microscopy, and X-ray diffraction.

A New Imaging Strategy for High-resolution Scanning Electron Microscopy of Biomass Specimens Using a Low-cost Ionic Liquid

Dian Yu

University of Toronto

Abstract:

Although biomass wastes, such as cotton, sawdust, and pinecone, are susceptible to electron beam damage and charging under high vacuum in a Scanning Electron Microscope (SEM), the issue can be alleviated using solutions of Room-Temperature Ionic Liquids (RTILs) with low vapour pressure and high chemical and thermal stability. The RTILs recommended in the literature are either expensive or hazardous due to the requirements of low viscosity, low density, and high hydrophilicity. Moreover, there has been no systematic study on the optimal imaging parameters accompanying this technique. This work demonstrates a novel approach of leveraging both the electrical conductivity of RTILs and the electron yield properties of biomass at a low acceleration voltage, enabling nano-scale morphological features to be imaged without artifacts.

Mechanically ground pinecone particles were treated with solutions of an inexpensive RTIL, 1-ethyl-3-methylimidazolium hydrogen sulfate ([EMI][HSO4]). Three types of solvents were used: DI water, methanol, and ethanol, each at concentrations of 7.5 vol% and 10 vol%. SEM images were obtained daily after the treatment for one week to identify the most effective formulation for the suppression of charging and permanence of electrical conductivity. Images of the ethanol-treated sample captured using different acceleration voltages and scan patterns were compared to the untreated ones obtained in variable-pressure imaging mode to quantitatively compare the spatial resolution and verify the features observed. X-ray Photoelectron Spectroscopy (XPS) was used to evaluate the effect of electron beam irradiation on the applied IL and provide insights to the interaction mechanisms.

In-situ Nanoindentation Characterization of Nano-grained Mg using Transmission Electron Microscopes

Guo-zhen Zhu

University of Manitoba

Abstract:
The direct microstructural observation of materials during deformation provides valuable insight into a deep understanding of the microstructure-mechanical property relationship. While the microstructural observation largely relies on morphological records of bright-field image sequences, additional crystallographic information makes it possible to investigate deformation processes, which are strongly affected by grain orientations, for example, grain rotation and grain boundary sliding during deformation. In order to achieve this, the hollow-cone dark-field imaging, with a tilted incident beam at a fixed angle, has been employed for in-situ nano-indentation testing. The tilted angle can be carefully chosen to track changes of selected crystallographic plane(s), or the key crystallographic features of grains. This method is applied to investigate the deformation mechanisms of nano-grained Mg. The intermediate grain size, with an average grain size of ~100nm, is used to study transition from grain-mediated deformation, the dominating mechanism of ultra-fine grains (tens of nanometers in diameter), to dislocation-mediated deformation, which largely determines the behaviors of coarse grains. The acquired hollow-cone dark-field images select all possible slip planes of Mg, and therefore, theoretically indicate the key crystallographic features for dislocations. Co-operative grain rotations and following dislocation movement has been observed while a qualitative analysis is still under investigation.

Posters:

A proposal to investigate the existence of dark matter using materials science

Thalles Lucas, Audrey Fung, Yilda Boukhtouchen, Sharlotte Mkhonto, Aaron Vincent, Joseph Bramante, Matthew Leybourne, Levente Balogh

Queen's University

Abstract:

Dark matter is one of the biggest mysteries in entire physics. Even though there are indirect proofs of its existence based on astronomical observations, it was not yet confirmed by direct experimental detection. The main cosmological models treat dark matter as a relic particle from the early universe, known as Weakly Interacting Massive Particles (WIMPs). There are several underground experiments trying to find a signal caused by WIMPs interaction with conventional matter. However, WIMPs present an extremely small cross-section for matter interaction rates, typically limited for 10 events per year in ton-scale detectors. One strategy to solve this problem is to work with minerals buried for billions of years. Paleo detectors could record nuclear recoil damage caused by dark matter interaction. WIMPs interactions are expected cause permanent damage in the shape of amorphous tracks in these minerals. Furthermore, the tracks caused by dark matter-induced nuclear recoils could be characterized using Transmission Electron Microscope (TEM) and Small-angle X-ray scattering (SAXS). For that purpose, we are proposing to work with two minerals: Olivine and Galena. The minerals will be subjected to proton irradiation at the Reactor Materials Testing Laboratory (RMTL), Queen's University, in order to emulate the nuclear recoils expected from WIMP interactions. The irradiated minerals will be inspected using traditional material characterization methods.

Production of Radiolysis-induced Bubbles in Deionized Water using Static Liquid Cell in Scanning Electron Microscopy

Mia San Gabriel, Stas Dogel, Hooman Hosseinkhannazer, Jane Y. Howe

University of Toronto

Abstract:

The expansion of liquid-based electron microscopy into scanning electron microscopy (SEM) applications is highly beneficial due to the SEM's capacity for larger volumes of liquid with easy sample preparation. However, the large interaction volume adds complexity to the way the electron beam interacts with the liquid. The electron beam induces the radiolysis of water, which results in the formation of gaseous bubbles upon hydrogen supersaturation. We herein report the immediate visual effects of these radiolysis-induced bubbles on the imaging of enclosed liquid in the SEM. Our studies were conducted using deionized (DI) water in a static liquid cell with electron transparent SiNx window chips optimized and manufactured by Norcada Inc. Each liquid cell has an approximate volume of 40nL. The liquid cells were imaged using a Hitachi SU7000 SEM with accelerating voltages of 3, 7, 10, and 15kV and respective beam currents of 311, 412, 489, and 623pA. DI water was observed to undergo several stages upon electron beam exposure. Initially the water appears still, then small bubbles form underneath the window and coalesce into a large gaseous region. The gaseous region grows until it rapidly transfers from the centre of the cell to the cell walls. Finally, the liquid boundary recedes and stabilizes with the DI water in the centre. We assumed that there is a thin layer of gas between the liquid and the window in this final stage. At 3kV, the bubble formation was significantly faster and occurred almost instantly upon exposure to the electron beam. We speculate that at low kV, the local density of radiolysis occurrences towards the surface of the liquid is greater than at higher kV due to a smaller interaction volume. This results in a faster increase in local hydrogen concentration and a shorter time period before supersaturation occurs and bubbles form.

Biomaterials

Oral presentations:

FEM Modelling of the Electrodynamic Responses in Rodent Brain Tissue under Stimulation with Metal and Hydrogel Materials

Jia Xi Chen

University of Toronto

Abstract:

There is an urgent demand to aid recovery in patients with neurological conditions such as Parkinson's disease, essential tremors, strokes, and epilepsy. Deep brain stimulation (DBS) offers a reliable solution with clinically shown effectiveness via the mechanism of inducing an electric field that activates the endogenous electrosensitive stem cells within the brain, encouraging permanent recovery. However, existing DBS electrode materials require further optimization in terms of geometry, mechanical and chemical properties, in order to minimize tissue damage upon electrode implantation and during stimulation. This study aims to select the experimental parameters that most effectively increase the proliferation and migration in neural precursor cells. Since the biological mechanism behind deep brain stimulation remains unknown, this study implements computational finite element models with COMSOL to optimize among six design prototypes, providing a fundamental understanding of the process from an electrodynamics aspect. The finite element method (FEM) model is applied to forecast the stimulation-induced current density and the time-varying electric field distribution within a homogenous, three-dimensional medium. This model is coupled to the equivalent Randles circuit model, which took one-dimensional input of the stimulation waveform to output the voltage across the bulk of the brain, accounting for electrochemical interactions at the electrode-brain interface. The outcome of this study is a proof of concept demonstrating the advantages of current-controlled source, non-insulated electrodes, and flexible non-metal electrodes during deep brain stimulation in rodents, essential for developing the next generation of novel electrodes by providing a guideline on desirable material candidates.

in situ formation of lipid-DNA particles using ultrasound and microbubbles for brain cancer characterization

Matthew Chen, Catherine Campbell, James Drake, Adam Waspe, Naomi Matsuura

University of Toronto

Abstract:

Tumours comprise of cells with mutated DNA. In brain tumours, cavitation of intravenously injected lipid-stabilized micron-scale bubbles (MBs) with focused ultrasound (FUS) can release brain tumour DNA into blood circulation. This DNA, acquired via a blood sample, can be used to identify specific mutations and select an effective treatment. However, this technique alone still results in low DNA levels, which can be confounded by DNA from other sources in the body. The lipid shell material of MBs may provide a new method for isolating tumour DNA. We hypothesize that cavitation of MBs with fluorescent dye and DNA can form self-assembled particles comprising lipids, DNA, and dye. These particles could then be sorted by fluorescence to collect tumour DNA.

MBs were made with lipids (DPPA, DPPC, DPPE-mPEG5k), glycerol, and C4F10 gas. DiI was included as a lipid stain. MBs (2x107/mL); DAPI-stained DNA (0.15mg/ml), as a tumour DNA proxy; and calcein dye (0.001mM); in saline were flowed (10mm/s) through a polyimide tube (ø: 1.1mm) w/o FUS (1MHz, 550kPa) treatment. MBs were characterized for size and concentration. Optical properties of particles were assessed with microscopy and flow cytometry.

FUS treatment of MBs (mode diameter: 2.0±0.2μm) increased ($p<0.001$) the population of lipid particles (0.5±0.2% to 10.2±1.2%) out of all particles detected. Particles with both DAPI-stained DNA and calcein also increased ($p=0.003$) from 0.3±0.2% to 1.0±0.2% with FUS treatment. DiI-stained lipid and DAPI-stained DNA were colocalized under microscopy.

FUS treatment increased the quantity particles expressing both DAPI and calcein, indicating DNA encapsulation. DiI and DAPI were colocalized under microscopy, indicating that MB lipids were associated with DNA. Results suggest that these fluorescent particles could potentially be used with optical techniques for isolation of these particles to collect brain tumour DNA. Future work will isolate and quantity DNA in sorted particles.

CaCO3 mineralized polyplexes for gene therapy

Teo Dick, Hasan Uludag

University of Alberta

Abstract:

Recently, it has been proposed that viruses benefit from the ability to self-mineralize under natural supersaturated conditions to increase robustness as an evolutionary advantage[1]. The protective effect of a mineral shell could provide increased chances for survival and improved infectivity [2]. Therapeutic applications using viral vectors for gene delivery have been demonstrated to benefit from mineralization due to the same mineral bio interactions [3–5]. Under the hypothesis that benefits from mineralization in viral gene delivery arise exclusively from mineral bio interactions (instead of virus capsid protein-mineral interactions), we presume the same benefits could be achieved with mineralized non-viral vectors, which are much safer. We tested this hypothesis by mineralizing pDNA/lipid-modified low molecular weight polyethyleneimines (PEI) polyplexes with CaCO3. The effect of mineralization and polyplexes composition on polyplex properties was evaluated by ELS, DLS, TEM, SEM, and gel electrophoresis. Then, in vitro GFP transfection efficiency was evaluated with flow cytometry for 2 different polyplex compositions and 9 different mineralizing concentrations. Mineralization at every concentration tested was capable of increasing the robustness of polyplexes even at highly dissociative conditions. However, calcium incubation also increased robustness at high concentrations, probably due to the formation of physical crosslinks with poly(aspartic acid). Gain of robustness through mineralization of calcium incubation seems to positively affect transfection efficiency in vitro. However, more tests are needed to find if other properties already reported for mineralized viruses could also be acquired by polyplexes.

Injectable Biodegradable Hydrogel Colloids for Osteoarthritis

Kierdra Dowling, Yu-Jack Shen, Camilo Barragan, Sebastian Mafeld, Naomi Matsuura

University of Toronto

Abstract:

Osteoarthritis (OA) is a chronic painful condition that affects approximately 303 million people globally. This condition creates a significant burden on the health care industry, with the economic burden of OA being estimated to be over $5 billion annually in Canada alone. In OA abnormal vessels develop around the affected joint driving inflammation, and aiding in the growth of new sensory nerves causing high levels of pain and disease progression. Previous work has shown that blocking the blood flow in these vessels reduces the patient's pain, restoring their quality of life. Existing clinical agents used in this procedure have many limitations such as polydispersity, causing unpredictable embolization, and permanent blockage, causing inflammation and damage to the surrounding tissues. Existing clinical agents are successful at treating OA of the knee, however, to advance this procedure to be used in OA of the hip or spine, a more controlled agent must be designed. Off target consequences in knee OA can cause skin discolouration and numbness and loss of function in the feet, however, due to the close proximity of vital organs to the hip and spine off target consequences in these areas could result in major damage to vital organs such as the kidneys. This research has developed a novel temporary embolic agent made from hyaluronic acid, a biodegradable polymer with the ability to decrease local inflammation. It has been designed to have a size range of 50 – 100 microns, matching the diameter of the neovessels, with a smooth hydrophilic surface to prevent aggregation in the catheter. This agent is also designed to have an elastic modulus ~30kPa to allow for the agent to be compressed down in the catheter, and to recover its size once in the vessel, thus avoiding catheter clogging. This precisely controlled embolic agent could enable safer and more effective embolization of OA in the knee, hip and spine.

Anisotropic Porous Collagen Scaffolds Towards Tissue Engineering

Kenneth Kimmins, Qin Wang, Christopher McCulloch, Eli Sone

University of Toronto

Abstract:

Tissue engineering scaffolds promote tissue regeneration by providing a structure where regeneration is encouraged. Collagen-based scaffolds are well-suited for this due to their similarities to many tissues. Anisotropy is a key consideration for tissue engineering scaffolds, as it can induce orientated collagen fibril production similar to native tissue. Porosity also plays an important role in guiding cell function and tissue regeneration. However, fabricating collagen scaffolds with both features is not easily achievable. Herein, we report a novel but simple fabrication method for such scaffolds by gas diffusion. Type I collagen dissolved in acetic acid were neutralized by ammonia vapours, resulting in scaffolds with aligned pores. Parameters related to the pH of the system were varied to explore ways to control porosity. Human gingival fibroblasts were seeded and cultured in the scaffolds pre-treated with fibronectin in vitro for up to 3 days, followed by DAPI and phalloidin staining to evaluate cell viability and morphology within the scaffolds. Acetic acid and ammonia concentrations both had significant effects in porosity. As the gelation time of the collagen increased by either increased acetic acid concentration or decreased ammonia concentration, pores became larger, but significantly fewer pores formed. Conversely, faster gelation time resulted in numerous small pores up to a certain point, beyond which generated fewer and larger pores again. It is hypothesized that pore formation is a result of phase separation by spinodal decomposition. The seeded cells formed long extensions, similar to the fibroblasts found in many native tissues. We are currently working on optimizing pore size (100–500 μm), and hypothesize that our optimized scaffold design will lead to cell alignment and in turn, oriented collagen production. The results of this work will provide new strategies for tissue engineering and regeneration.

Using acid catalysis to accelerate binder setting in bioactive glass composite bone tissue scaffolds

Marzieh Matinfar, John Nychka

University of Alberta

Abstract:

Currently, bone reconstruction techniques are mainly based on the use of tissue grafts and artificial scaffolds. Due to the immunological, structural and volume limitations of natural bone grafts, bone-grafting procedures are being gradually shifted to synthetic bone substitutes. Bioactive glasses (BG), such as 45S5, have appealing characteristics as a bone scaffold material due to their osteoconductivity, biodegradability, and ability to induce new bone formation. However, we found three main challenges in common techniques for processing BG materials into bone scaffolds: (1) the need for heat treatment; (2) lack of formability; (3) the need for 3D models and imaging. This research seeks to develop a new processing route for fabricating BG bone scaffolds. The design approach builds on our recent proof-of-concept work aimed at creating a formable scaffold composite by mixing 45S5 BG powder and a sodium silicate binder solution, which self-sets in air. The main driver of this work is to reduce the binder setting time to a range that is practical for clinical applications. This work investigated three different methods to accelerate binder setting time through acid catalysis: (1) exposing the scaffolds to high-purity CO2 gas (i.e., in situ formation of carbonic acid); (2) adding boric acid; and (3) adding phosphoric acid. Preliminary experiments revealed reduced setting times from 10 days to 2-20 minutes. The setting reaction and its by-products have been studied using Raman spectroscopy and x-ray diffraction (XRD). The effect of CO2 gas flow rate (method 1) and the concentration of acid solutions (methods 2 & 3) on the setting time and compression strength of composites was determined. The long-term objective is to determine the optimum setting method to minimize setting time whilst producing a bone scaffold with maximum compressive strength. Further development will involve in vitro and in vivo studies to develop a prototype kit for use in an operating room.

Contrast Enhanced Ultrasound for Cancerous Lymph Node Detection and Staging

Sean McGrath, Masato Aragaki, Alexander Gregor, Yamato Motooka, Yu-Jack Shen, Matthew Chen, Nicholas Bernards, Kazuhiro Yasufuku, Naomi Matsuura

University of Toronto

Abstract:

Lung tumours are one of the most common types of cancer. These tumours commonly spread to lymph nodes before other areas, making lymph nodes around the cancer important to sample for diagnosis. This is accomplished using a bronchoscope, a device inserted through the mouth and into the trachea for sample collection. A special ultrasound probe, known as an endobronchial ultrasound (EBUS), can be equipped to the end of the bronchoscope to help with proper biopsy collection. Ultrasound contrast imaging with microbubbles (MBs) is commonly employed to diagnose other cancer types, where it is used to identify features of the lymph node that would not be otherwise apparent by conventional ultrasound imaging (i.e. blood vessels). However, MBs have yet to be used with lung tumours due to the ultrasound-reflective properties of gas-tissue interfaces. This study explores the use of contrast-enhanced EBUS and its ability to detect MBs. EBUS (Olympus, Japan) was evaluated in comparison to clinical and preclinical contrast-enhanced ultrasound systems. In vitro, various concentrations of MBs were flowed through a vasculature-mimicking flow phantom. Both EBUS and the clinical ultrasound system (operated at a similar frequency and pressure) were used on the flow phantom, with the resulting image intensities averaged over a region of interest. This indicated the useful range of microbubble concentration for both ultrasound systems. Stability testing of the MBs at 37 ºC in phosphate buffered saline showed no significant difference between the relative brightness captured by the two ultrasound systems. In vivo, the EBUS was used simultaneously with a preclinical ultrasound system on a mouse model of lung cancer, to assess the ability of EBUS to detect tumour vasculature. Despite the preclinical ultrasound system operating at a much higher frequency than EBUS (18 MHz), the preclinical ultrasound and EBUS yielded tumour brightness curves with a strong correlation coefficient of R=0.967.

Novel Morphologies of Mesoporous Hierarchically Assembled Nanostructured Hydroxyapatite Particles: Influence of Some Synthesis Conditions

Ravinder Pal Singh, Anoop Aggarwal, Amardeep Singh Kang

Lovely Professional University, Phagwara, Punjab, India

Abstract:

Hierarchically assembled nanostructured apatitic (HANA) particles with mesoporous structure have been acclaiming potential drug delivery systems owing to their novel morphologies and unique textural properties. On the other hand, synthesis of HANA particles involves intricate procedures and synthesis process parameters play critical role in their formation. This investigation systematically evaluated the influence of both temperature and duration of hydrothermal heating on the architecture and other physicochemical properties of HANA particles. Variation in temperature and duration of heating unfolded variety of HANA particle morphologies including bundle-like, flower-like, dumbbell-like and spherical ended dumbbells-like particles. All HANA particles were phase pure apatitic particles with varied degree of crystallinity and lattice strain. Phase, molecular and elemental structures corroborated apatitic formation in all particles. Isotherms confirmed the mesoporous structure of all HANA particles with surface area and pore volume varied between 16-23 m2g-1 and 0.009-0.048 cm3g-1, respectively. On the basis of ionic release rate, drug loading and release rate testings; spherical ended dumbbell-like particles exhibited superior drug loading efficiency and sustained drug release rate in simulated body conditions. Therefore, amalgamation of such novel properties, such HANA particles can be employed for multifunctional therapeutic applications including drug delivery and tissue regeneration agents.

Mechanisms of Microbial and Viral Attachment to Limited-Area Superhydrophobic Topographies

Desmond van den Berg, Dalal Asker, Ben Hatton

University of Toronto

Abstract:

Healthcare-associated infections (HAI) affect 1 in 20 patients admitted to a hospital and represent nearly 10% of total inpatient costs – amounting to an annual economic burden exceeding $35 billion to global health systems. In health care settings, high-touch surfaces have the greatest degree of microbial contamination and transmission. One strategy implemented we have implemented is the application of superhydrophobic topographies, though little is understood about the mechanisms of microbial attachment to these types of surfaces. Our objective is to understand the attachment to such surfaces, to better understand the design parameters for successful topographies. In this work, we investigate rates of microbial and viral adhesion to superhydrophobic elastomers molded with micro- and nanopost arrays, where we test the role of micropost size relative to microbial cell size. This was achieved through the molding of microtopographies (generated via photolithography) ranging from 0.5 to 150 micrometers in diameter in a UV-curable polyurethane compound. After chemical functionalization to impart a superhydrophobic behaviour to these topographies, we found the adhesion of three bacterial strains (S. aureus, P. aeruginosa, and E. coli), a yeast (C. albicans), and two seasonal coronavirus strains (OC43 and 229E) could be reduced by factors of 103 to 104. Using these surfaces, comparisons of the mechanism for microbial attachment to limited-area superhydrophobic topographies to existing physical models could be assessed, for which the random sequential adsorption (RSA) proved to be most promising. With this knowledge, ways in which surfaces could be engineered to prevent attachment and transmission are better understood.

Posters:

Nanoscale phospholipid-stabilized drug-loaded bubbles for ultrasound-triggered cancer therapy

Patrick Dong Min Chang, Yiran Zou, Yun Xiang, Sharshi Bulner, Alex Wright, Dr. David E. Goertz, and Dr. Naomi Matsuura

University of Toronto

Abstract:

Introduction: Biocompatible phospholipids can be formulated with anticancer drug molecules into ultrasound (US)-responsive drug-loaded microbubble contrast agents. These bubbles can then be inertially cavitated (i.e. imploded) for subsequent triggered release at therapeutic targets of interest. Here, we exploit the higher surface-area-to-volume ratios of nanomaterials for enhanced drug loading capacities, introducing US-triggered drug-loaded nanoscale bubbles for localized cancer therapy in vivo.

Methods: Phospholipid (DPPA, DPPC, DPPE-mPEG5k)-stabilized drug-loaded nanobubbles (NBs) were assessed for in vitro size and stability at 37°C. Drug loading was assessed via liquid chromatography-mass spectrometry. In vitro cytotoxicity was examined on murine breast cancer EMT-6 cells using an MTT assay with samples cavitated under US pressures of 0.25-1.36 MPa. In vivo NB circulation lifetimes were assessed by contrast-enhanced ultrasound (CEUS) using a clinical US scanner on EMT-6 tumour-bearing mice models.

Results: 106±16 μg of the drug ($n \geq 6$) was loaded onto ~1010 bubbles (mode diameter of 230 nm; 99.5% of bubbles ≤1μm) per ~0.4 μL of gas ($n \geq 9$). NBs were more cytotoxic than the free drug alone with no US exposure in vitro and the most cytotoxic effects were exerted upon exposure to US pressures of 1.36 MPa. NBs can be monitored via CEUS with circulation lifetimes of ~5 min in vivo.

Conclusions: NBs offer drug doses of ~2.5 mg/kg (following a reported safe-for-injection gas dosage of 9 μL/kg), comparable to the highest approved dose of the clinical drug formulation. US exposure of NBs can enhance in vitro cytotoxicity compared to NBs with no US stimulation and trigger drug release from NBs. CEUS imaging can be coupled to monitor real-time US-triggered NB destruction in vivo. Future work will assess the in vivo biodistribution of NBs with US pulsing parameters for drug delivery and vascular disruption regimes in preclinical breast cancer mice models.

Biomimetic Collagen Mineralization

Liyang Zhong, Ruixin Gao

University of Toronto

Abstract:

Collagen is a fibrillar structural protein that is found in mineralized tissues, such as bone and dentin. The biomineralization of collagen plays a critical role in the tissue formation process; however, it is not fully understood due to its complexity. To date, researchers have successfully developed in vitro models that can reproduce intrafibrillar mineralization as well as aligned hydroxyapatite (HA) minerals within the fibrils, which are both distinctive properties of natively mineralized collagen. A key characteristic that has not been extensively studied is the preferential distribution of the HA crystals in the gap regions of collagen fibrils, revealing a banded pattern. Yet, it is crucial to reproduce this property since the distribution of the crystals may affect the mechanical properties of the fibrils. Here we report on an in vitro model that can highly mimic native collagen fibrils, which will accelerate the development of novel bioinspired collagen-based materials and scaffolds for tissue repair and regeneration applications.

Our in vitro model shows that mineralization of chemically crosslinked collagen fibrils results better alignment of HA crystals and a clear banding pattern, similar to native collagen. Even though it has been reported that crosslinking affects the mechanical properties and stability of the collagen fibrils, the mechanism behind how crosslinked fibrils can produce such banded pattern is unknown. In this study, our objective is to investigate how crosslinking changes the stiffness and charge of collagen and determine their relative contribution to the mineralization of collagen fibrils. This objective is achieved through various methods and degrees of crosslinking, colorimetric assays, as well as characterization techniques such as transmission electron microscopy (TEM) for qualitative measurement, and atomic force microscopy (AFM)-nanoindentation for determining the mechanical properties of the fibrils.

Computation and AI

Oral Presentations:

Pushing the length and time scales of AIMD

Daniel Abarbanel, Hong Guo, Peng Kang, Zimin Feng

(McGill University, Hydro Quebec)

Abstract:

"Molecular Dynamics (MD) is a commonly used technique to simulate the evolution of atomic structures and complex materials. MD based on classical force fields can solve large systems with relatively long time scales. Since the accuracy of MD depends on the quality of the underlying force fields, and there are many situations where complex chemical reactions occur due to electronic interactions, an important research direction is to advance the method of Ab Initio Molecular Dynamics (AIMD) based on the self-consistent Kohn-Sham density functional theory (KS-DFT), to larger length and time scales.

In this work, we present an accelerated AIMD which harnesses its power by two approaches. First, the AIMD is based on our real space KS-DFT method RESCU [1] which can efficiently solve supercells containing many thousands of atoms. Second, we leverage Gaussian Process Regression (GPR) to efficiently extrapolate forces by interpolating between KS-DFT calculations from previous timesteps in the AIMD simulation. By extrapolating forces via GPR when possible, and only calculating forces via KS-DFT when necessary, novel reactive dynamics on increasingly large timescales can be studied using modest computational resources. The accelerated AIMD is applied to simulate the Solid Electrolyte Interphase (SEI) formation in a 2590-atom system consisting of an interface between a lithium slab and liquid organic electrolyte, to time scales of a picosecond or more, where important chemical reactions at the solid/liquid interface are identified.

[1] Vincent Michaud-Rioux, Lei Zhang, and Hong Guo, J. Comput. Phys. 307, 593 (2016)."

Edge Dislocation Mobility in NbMoTaW, Body Centered Cubic High Entropy Alloy

Abu Anand, Prof. Chandra Veer Singh

(University of Toronto)

Abstract:

In this work, we try to understand the mobility of ½ <111>{112} edge dislocations in NbMoTaW, a comprehensively understood single phase bcc HEA system using classical Molecular Dynamics. Pierels stress for the HEA system is around 600 MPa where the dislocations are immobile (Region I). Region I is barely observed for the component elements. Once the dislocation starts to move in the HEA, the velocity increases exponentially for a small stress range (Region II) and then becomes linearly dependent on applied stress (Region III). The stress at which the the transition from region II to region III happens is changing with temperature suggesting a thermally activated mechanism of motion. Although, the linear regime appears to be independent of the temperature, consistent with viscous damping dynamics. In crystals the resistance to dislocation motion primarily arises from the lattice vibrations. These vibrational modes represented by phonons and the damping force from phonons balances the Peach-Koehler force on the dislocations. The phonon spectrum broadens for the HEA system and there is a peak shift to the lower frequency region owing to its chemical complexity. Shift in phonon peaks to a lower frequency compared to the component elements increases the drag force for dislocations. Nudged Elastic Band calculations reveals a ragged energy pathway for the dislocation motion. Dislocation mobility trends in HEA could be attributed to the increased phonon drag and the solute pinning offered by the components in the HEA.

NIST-JARVIS Infrastructure to Enable Deep Learning and Quantum Computation Methods for Improved Materials Design

Kamal Choudhary

(National Institute of Standards and Technology)

Abstract:

We'll discuss deep learning methods 1) Graph neural network (GNN) for improved atomistic material property predictions of solids and molecules, 2) Convolutional neural network for STM and STEM image related tasks, and 3) quantum algorithm method: Variational Quantum Eigensolver (VQE) for predicting electron and phonon properties. Many GNN models for atomistic property predictions are based on bond-distances mainly. We developed Atomistic Line Graph Neural Network (ALIGNN) that performs message passing on both the bond-distances as well as bond-angles. We apply ALIGNN to train 60 material property models in the Materials Project, JARVIS-DFT, hMOF and QM9 datasets leading to up to 44 % improved performance compared to previously known GNN methods. Next, we'll discuss the AtomVision package which can be used to generate scanning tunneling microscope (STM) and scanning transmission electron microscope (STEM) datasets. Then we apply deep learning frameworks for image classification and defects detection tasks for 2D materials. Currently, the application of quantum algorithms such as VQE is mainly limited to molecules. We'll show using tight-binding approaches for electrons and phonons, quantum circuit-based methods can be applied for solids using AtomQC package. All of the above projects are part of the NIST-JARVIS infrastructure (https://jarvis.nist.gov/).

Hybrid Composite Fiber Orientation and Topology Optimization using Contour Based Fiber Mapping

Andrew Cross, Craig Steeves

(University of Toronto Institute for Aerospace Studies)

Abstract:

Generating lightweight, stiff structures is a common design problem for a variety of industries. To address this, several techniques have been developed to generate such structures for conventional isotropic materials, including numerical techniques such as topology optimization. As the mechanical properties of orthotropic materials, such as fiber reinforced composites, often provide superior performance compared to isotropic materials, it is desirable to extend numerical optimization to composites. With advances in manufacturing techniques, such as automated fiber placement, continuous fiber paths can be fabricated in laminates with complex geometry, as produced by topology optimization. To model complex fiber paths, contour based fiber mapping is utilized. This method uses the contours of a generating function to define the fiber orientations, while the basis function parameters are treated as design variables. A modified version of the solid isotropic material with penalization method is utilized to perform topology optimization. The flexibility of the method is demonstrated using a series of 2D test cases while its performance is evaluated using results from equivalent isotropic materials. Considerations for setting the constant basis function parameters as well as strategies for decreasing the number of elements with intermediate density in the final topology are also discussed.

Stacking fault and martensite transformation mediated plasticity in high entropy alloys studied by atomistic simulations

Chuang Deng, Jianwei Xiao

(University of Manitoba)

Abstract:

High entropy alloys have attracted significant attention in recent years due to their unique plasticity as compared to conventional metals. In this talk, we present the findings based on the well-studied Cantor alloy, CoNiCrFeMn, by using atomistic simulations regarding the underlying deformation mechanisms in both bulk nanocrystalline and nanowire forms. It is found that the plastic deformation of nanocrystalline CoNiCrFeMn HEAs is dominated by a partially reversible FCC to HCP martensite transformation mediated by stacking faults and partial dislocations, which is dramatically different from the full dislocation and deformation twinning dominated plasticity in conventional FCC metals. In contrast, the martensitic transformation in CoNiCrFeMn nanowires was found to be reversible upon reverse loading, thus enabling shape memory effects in them. Those mechanism are found to be strongly associated with the metastable nature of CoNiCrFeMn, whose stacking fault energy can be easily tuned by varying its compositions. Those findings are in excellent agreement with recent experiments.

Atomic-Scale Investigation of the Shock Response of Polymers

Nuwan Dewapriya, Ron Miller

(Carleton University)

Abstract:

"Recent advances in experimental techniques have allowed us to explore the behavior of materials under extreme dynamic conditions. For example, laser-induced projectile impact tests have revealed that the specific penetration energies of ultrathin polymer films are remarkably high compared to conventional protective materials. However, the current experimental techniques cannot elucidate some of the complex energy dissipation mechanisms, which can only be realized through atomistic simulations.

We conducted molecular dynamics (MD) simulations of plate impact tests to obtain molecular-level insights into the shock response of three amorphous polymers (polyurea, polyurethane, and polyethylene). First, we examined the fidelity of a non-reactive MD force field by comparing its predictions with available experimental data and conducting density functional theory calculations. The subsequent plate impact test simulations allowed us to test two common assumptions associated with the interpretation of plate impact experiments. We found that the commonly used free surface approximation can underpredict the shock pressure in the polymer. Moreover, the spall strength computed from the free surface velocity history can be significantly smaller than the actual tensile stress in the region of spallation."

Theoretical investigation of charge and neutral vacancy diffusion in anatase (101) surface using activation relaxation technique coupled with *ab initio* method.

Jeffrey Roshan De Lile [1] and Normand Mousseau [1,2]*

[1] Department of Physical Engineering, Polytechnique Montréal, Case postal 6079, Station Centre-Ville, Montréal, QC H3C 3A7, Canada.

[2] Succursale Centre-Ville, Département de Physique, Université de Montréal, Case Postale 6128, Montréal, QC H3C 3J7, Canada.

Abstract:

The low friction of 2D materials allows their application as solid lubricants, with graphene and MoS2 being the most studied cases. However, MXenes, despite representing one of the emerging classes within this family of nanomaterials and having a wide range of promising applications, have only been scarcely studied for lubrication. In this work, the friction properties of Ti3C2Tx MXenes is investigated by Friction Force Microscopy (FFM) with a sharp diamond tipped cantilever. Furthermore, Density Functional Theory (DFT) is used to calculate the Potential Energy Surface (PES) of MXenes with different surface coverages, including both homogeneous and heterogeneous passivation schemes. While other 2D materials present layer dependent friction properties and thus require multilayer systems for lubrication, MXenes presented the same friction coefficient at mono, bi and trilayer, which makes them uniquely promising as solid state lubricants at monolyer thickness. DFT assigned this behavior to MXenes having higher binding energy and activation barrier for interlayer shear than graphene, causing its friction behavior to be controlled by the diamond-MXene interface. DFT also estimated that OH termination induces higher binding energy due to the formation of hydrogen bonds, which results in a more corrugated PES and higher friction. Therefore we propose annealing as a method for enhancing the lubricating properties of MXenes, as it favoured O and F terminations and caused a reduction of 16-57% in friction, in accordance with the 34% estimated by DFT with similar heterogeneous coverages. Overall, we demonstrated for the first time that the lubricating properties of MXenes are uniquely placed among 2D materials in terms of mechanisms and capabilities, with low friction at the monolayer scale which can be further reduced by annealing.

Fe-containing Al Alloys for Applications in Electric Vehicles

Henry Hu

(University of Windsor)

Abstract:

Iron is the main component of the earth's core, the most abundant element on the earth (about 35%), and it is relatively high in the sun and other stars. Also, it is a common and cheap metal in the manufacturing industry. Recently, with the rapid development of electric vehicles, more and more automotive companies are willing to develop new lightweight material for electric motors used in electrical vehicles. The iron–containing aluminum alloys can be considered as a good candidate, due to its great strength and electricity performance. This review describes various properties of aluminum-iron alloys including mechanical properties and electrical conductivities, as well their relation to the Fe contents. Also, metallurgical aspects of aluminum-iron alloys, including phase diagrams, equilibrium and non-equilibriun solidification, microstructure development, and castability. The further research and development work are outlined in terms of developing aluminum-iron alloys for some potential and value-added automotive applications.

A new approach to assess the role of kinetics on the Precipitation Hardening of Al-Cu Alloy

Seyed Sajjad Jamali, Daniel Larouche, X. Grant Chen

(Laval University, The University of Quebec at Chicoutimi)

Abstract:

Precipitation hardening of different phases of Al−Cu alloy is analyzed in the mixed-mode regime employing computational analysis. Kinetical pathways and thermomechanical principles were taken into account based on the complementary theory of solid-state nucleation and growth to assess the role of interfacial mobility on the evolution of different types of precipitates (θ'', θ' and θ). Based on the collective phenomena of nucleation, this model indicates that different phases' embryos are available in the matrix from the earlier stage of the procedure, and the interfacial mobility manages their velocity through the growth and dissolution. All phases are in competition, and the reason explaining why some phases grow before others is their favorable kinetics. The overall precipitation strengthening relies on the geometrical parameters of these phases, particularly their size, shape, and volume fraction at any given time. Size and volume fraction of various precipitates are computed in the shape-preserving mixed-mode model from the earlier nucleation stage to the equilibrium state of microstructure evolution. This information was used to estimate the critical resolved shear stress of different phases and their contribution to the total precipitation strengthening based on the shearing and Orowan looping mechanisms.

Enhancements to the Mould Water Model Physical Twin of a Continuous Steel Slab Caster for Machine Learning Development

Jackie Leung, Soumitra Dinda

(University of Toronto)

Abstract:

The continuous slab casting machine is a major component to the overall steel manufacturing process. In the Continuous Casting (CC) process, liquid steel is transported into a mould where solidification initiates and continues down the length of the CC machine. Steel slabs are produced, which subsequently get rolled into coils that are eventually further processed into consumer products. Disruptions to fluid flow in the CC mould can result in slab defects, compromising quality for final products. Steelmakers continually strive to increase productivity without compromising quality through process improvements. A challenge to achieving this goal is that liquid steel inside the mould cannot be directly observed. One method to understand fluid flow phenomena has been through simulations by physical modelling. A full-scale mould water model, or physical twin, at the Process Metallurgy Research Lab is used to study fluid flow phenomena in the CC process. At present, sensors and video cameras installed in the physical twin provide a mix of abundant quantitative and qualitative information during experiments. In the modern digital age, application of machine learning techniques in heavy industry has become more mainstream. A new challenge presents itself: How can machine learning be incorporated into physical modelling to derive further insight to help improve the real CC process. In this presentation, it will be discussed how novel computer vision techniques are being developed and applied to convert the qualitative information into digital data, which in turn will be used to feed into machine learning algorithms, with the purpose of deriving further insight to make improvements for the real industrial process.

First principles-based prediction of composition-dependent atomic diffusion in paramagnetic Fe-Ni solid solutions

Kangming Li, Chu-Chun Fu

(Université Paris-Saclay, CEA, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France)

Abstract:

"Atomic diffusion plays a key role in controlling the kinetics of microstructural evolution. Diffusion in Fe-based alloys can be highly sensitive to the magnetic state [1], but an accurate consideration of finite-temperature magnetic effects is challenging, especially for concentrated magnetic alloys.

Here we focus on the fcc Fe-Ni system, which is a prototype of austenitic alloys and is paramagnetic in typical conditions. Vacancy-mediated diffusion is investigated for the whole composition range, via kinetic Monte Carlo simulations based on a first-principles parametrized effective interaction model. With an explicit consideration of magnetic excitations and magnetochemical interplay, our approach is shown to provide an accurate description of phase stability and vacancy formation properties of fcc Fe-Ni alloys [2,3].

The predicted tracer diffusion coefficients D* are in good agreement with experimental data, confirming a weak composition dependence in thermal equilibrium conditions. The concentration dependence of D* is analyzed in terms of its constituents, namely equilibrium vacancy concentration, jump frequency and kinetic correlation factor. We show that simply adopting magnetic ground states, as often done in previous studies, can lead to large overestimation of D*. We also discuss our prediction of diffusion under non-equilibrium conditions (e.g., under irradiation).

[1] A. Schneider et al., Phys. Rev. Lett. 124, 215901 (2020).

[2] K. Li et al., Phys. Rev. B 104, 104406 (2021).

[3] K. Li et al., arXiv:2203.04688 (2022).

Localization model description of the interfacial dynamics of crystalline and metallic glass thin films and nanoparticles

Gazi Mahmud, Hao Zhang, Jack Douglas

(University of Alberta)

Abstract:

Any amorphous structure below its melting point, also known as supercooled liquid (SCL), progressively relaxes to a lower free energy state and finally becomes metastable SCL. Determining the relaxation time of amorphous material is important for tempering, annealing and other industrial applications. The rate of relaxation is temperature-dependent and can be minutes at lower temperatures. Therefore, finding relaxation time can be difficult and computationally expensive. On the other hand, Debye-Waller factor (DWF), or the mean square particle displacement <u2> on a ps 'caging' timescale is easy to compute numerically or determine experimentally. Localization Model (LM) description, without any free parameters, can relate DWF or <u2> to the structural relaxation time (τα). When combined with the 'decoupling' or Fractional Stokes-Einstein relation linking τα to diffusion coefficient (D), the localization model also allows for the prediction of the diffusion coefficient D from <u2>.

A recent study of structural relaxation in Cu–Zr metallic glass materials having a range of compositions and over a wide range of temperatures proved that the Localization Model description can relate <u2> to τα and D, without any free parameters. Later, the relation between <u2> and τα in crystalline UO2 under superionic conditions confirmed the generality of this model. In this study, we found the LM model also describes the interfacial dynamics of model crystalline metal (Cu) and metallic glass (Cu64Zr36) thin films and crystalline metal (Cu) and metallic glass (Cu64Zr36) nanoparticle to a good approximation, further confirming the usefulness of the model. We also show that the Tammann temperature, where the mobile interfacial layer starts to initiate, can be estimated precisely for both crystalline and glass-forming solid materials from the condition that the <u2> of the interfacial region and <u2> of the material interior coincide.

A local basin approach to the kinetic activation-relaxation technique

Md Mijanur Rahman, Normand Mousseau

(Université de Montréal.)

Abstract:

Kinetic Monte Carlo (KMC) simulations can become inefficient in the presence of low-energy barriers that dominate the kinetics, as each step is then associated with a very small clock increase. In some cases, these events are flickers, a set of states, separated by low-energy barriers deep in a energy basin and that do not contribute to the evolution of the system. We propose a local basin kinetic Activation-Relaxation Technique algorithm (kART), an off-lattice KMC algorithm with on-the-fly event cataloging, to compute on-the-fly statistically exact analytic solution of the connected flickering states and their escape rate as the energy landscape is explored, at the cost of specific trajectories using basin-auto-constructing Mean Rate Method (bac-MRM), a master equation-like approach based on mean-rate method that classifies the energetic landscape in basin states and non-basin states [1]. In this presentation, we will discuss in detail about the implementation of the local basin kART simulations that contain local basins and non-basin events simultaneously. We also review the time distribution of basin escapes and interactions between basin and non-basin states.

[1] B. Puchala, M. L. Falk, and K. Garikipati, An energy basin finding algorithm for kinetic Monte Carlo acceleration, J. Chem. Phys. 132, 134104 (2010).

Activation-relaxation technique with machine learning on-the-fly

Eugene Sanscartier, Normand Mousseau

(Université de Montréal.)

Abstract:

Diffusion processes, evolution of defects in crystals and relaxation of disordered materials can be understood through a detailed description the energy landscape for these various systems. To construct this description, it is necessary to turn to methods such as the activation-relaxation technique nouveau (ARTn) [Barkema GT, Mousseau N. Phys. Rev. Lett. 1996;77(21):4358] that explore the energy landscape with an efficient search algorithm for identifying and reconstruction activated mechanisms and evolution pathways.

Even for methods such as those, exploring the energy landscape requires considerable effort: generating a single activated event in a complex system can require many hundreds of force evaluations. If this is within the realms of ab initio description for small systems with a restricted set of relevant activated mechanisms, it is necessary to turn to empirical potential for more problems of interest. Yet, empirical potential are notoriously unreliable for complex environments and resulting descriptions are essentially qualitative.

To overcome this limitation, we present here an on-the-fly machine learning approach for generating potentials able to describe complex environment as, due to the nature of the landscape explored and the steps involved to push a system, upstream work on the data generation might still be insufficient, extrapolating outside of its learned domain. This approach builds on the linear expansion in the basis of moment tensor approach developed by Alexander Shapeev and collaborators. [Podryabinkin EV, Shapeev AV. Comput. Mater. Sci. 2017;140:171-80]

Here, we demonstrate the interest of this method by looking at simple test systems including vacancy diffusion in Si.

Towards experimentally and theoretically consistent electronic structure calculations of solvated ions: a density functional theory study

Javad Shirani, Sinan Abi Faraji, Shuaishuai Yuan and Kirk H Bevan

(McGill University.)

Abstract:

Solvated transition metal (TM) ions play an important role in the operation of energy storage systems, including redox flow batteries and associated applications. In order to engineer the performance of such energy storage devices, a fundamental understanding of the electronic structure of solvated species is needed to predict and engineer accessible redox energies for energy storage. However, no theoretical framework currently exists which can accurately predict the redox energies of solvated species from first-principles – in the absence of experimentally benchmarked parameters. To address this shortcoming and further enable the accurate prediction of solvated redox energies, we investigate the electronic structure (redox energies) of aqueous ferrous and ferric iron. From this model system, for which accurate state-of-the-art experimental spectra exists, we are able to resolve two main challenges in accurate prediction of solvation energies. The first challenge arises from the accurate treatment of exchange-correlation interactions following from the general form of Koopmans' theorem. The second challenge arises from the elimination of finite size errors arising from the ionically charged nature of such solvation calculations. Using a combination of classical molecular dynamics and exchange tuned hybrid functional calculations, our findings point towards the need for the development of a model that can capture the coupled polarization interaction between nuclear and electronic degrees of freedom, while also satisfying the redox energetics required by the general form of Koopmans' theorem in density functional theory. The outcome of this work is a closer correspondence between theoretical predictions and experimental measurements, while retaining consistency in the theoretical approach without empirically tuned parameters. This avenue of exploration is expected to further the predictive design space of redox energies in energy storage engineering.

Learning the atomic energy in grain boundaries by a simplified descriptor

Xinyuan Song, Chuang Deng

(University of Manitoba)

Abstract:

With the development of machine learning (ML), lots of complicated descriptors have been developed to represent local atomic environments (LAEs) in the material. Among them, the smooth overlap of atomic positions (SOAP) vectors shows excellent performance in representing chemical LAEs and learning atomic energies. However, SOAP vector contains hundreds of features which makes it uninterpretable and hard to extract useful information from ML model. In our study, we propose a route to simplify the SOAP vector and found that a few features of SOAP vector contain most of the energetic information of GB atoms. We used simplified descriptor to learn atomic energy of GB atoms in 172 Al and 388 Ni coincidence site lattice GBs as well as general GBs in the nanocrystalline models by linear regression ML algorithm and found that, compared to traditional descriptors such as Voronoi index, excess volume, centrosymmetry, or local entropy, the simplified descriptor shows higher predictive fidelity with only 2-5 features. The simplification method is also believed to be appliable in learning other LAE related GB properties such as thermal conductivity or magnetic movement of GB atoms. A simple and efficient descriptor of the LAE should allow us to have a clearer picture of the structure-property correlation in GBs, which is essential for GB engineering.

Phase field investigation of anisotropic grain growth

Ayush Suhane, Matthias Militzer

(The University of British Columbia)

Abstract:

Migration of grain boundaries (GB) during recrystallization and grain growth plays a crucial role in modifying the microstructure which determines the physical and mechanical properties of a material. The grain boundaries are anisotropic in nature and may have for example GB mobilities which vary within orders of magnitude as a function of GB structure. Presence of solutes further complicates the microstructure evolution as grain boundary migration rates are influenced by solute segregation due to the solute drag. Solute segregation energies depend also on the GB structure such that mobility anisotropies may be magnified by solute drag anisotropies. Here, phase field simulations with anisotropic GB properties are conducted to quantify the resulting grain growth kinetics. A critical discussion will be presented to identify the limits where a representative grain boundary can be defined that can be used in phenomenological grain growth models. Within these limits, a representative segregation energy for solute elements informed from DFT simulations will be used to identify the candidate solute elements that may promote grain refinement in steels and tungsten, respectively.

Evolutionary neural network approach simulates large-scale high-entropy alloys

Conrard Tetsassi Feugmo

(National Research Council of Canada)

Abstract:

High-entropy alloys (HEAs) are particularly interesting because of their energy-related applications. Computational modeling is necessary for targeted and rapid HEAs discovery and application, and constructing an appropriate atomic structure is the first step towards reliable predictions of materials properties. We propose a method of neural evolution structures (NESs) combining artificial neural networks (ANNs) and evolutionary algorithms (EAs) to generate High Entropy Alloys (HEAs) structures. Our inverse design approach is based on pair distribution functions and atomic properties and allows one to train a model

on smaller unit cells and then generate a larger cell. With a speed-up factor of approximately 1000 with respect to the Special quasi-random structures (SQSs), the NESs dramatically reduces computational costs and time, making possible the generation of very large structures (over 40,000 atoms) in few hours. Additionally, unlike the SQSs, the same model can be used to generate multiple structures with same fractional composition. A number of NE structures have been used to compute selected properties such as the elastic constants, the bulk modulus, and the Poisson ratio, and the results are similar to those of structures generated with SQS.

Conrard Giresse Tetsassi Feugmo, Kevin Ryczko, Abu Anand, Chandra Veer Singh, and Isaac Tamblyn , ""Neural evolution structure generation: High entropy alloys"", J. Chem. Phys. 155, 044102 (2021)

A first-principles study of solute-grain boundary segregation in a Ti-Mo alloy

Hariharan Umashankar, Daniel Scheiber, Vsevolod Razumovskiy and Matthias Militzer

(The University of British Columbia)

Abstract:

Solute segregation in alloys is a key phenomenon which affects various material phenomena such as embrittlement, grain growth and precipitation kinetics. In this work, we study solute segregation of Y, Zr, and Nb to a Σ5 BCC grain boundary in Ti-25 at % Mo using density functional theory (DFT) calculations. The Ti-Mo alloy was selected as BCC-Ti is unstable at 0 K. We lay out a systematic approach by computing the solution energy distributions in the bulk alloy constructed using Warren-Cowley short-range order parameters to find a representative bulk-solute reference energy. Additionally, we consider different scenarios of a solute atom replacing different sites in terms of their local Ti-Mo chemistry at the GB plane to calculate a distribution of binding energies. Further analysis shows that these binding energy trends can be rationalized based on solute volume and the excess volume of grain boundary sites, i.e. a primarily elastic interaction. Thus the segregation energies scale with the solute size such that Y has the largest segregation energies followed by Zr and Nb.

Hybrid Model for Endpoint Prediction in Basic Oxygen Furnace

RuibinWang

(University of Toronto)

Abstract:

Strict monitoring and prediction of endpoints in Basic Oxygen Furnace (BOF) is essential for end product quality and overall process efficiency. Existing control models are mostly developed based on thermodynamic principles or by deploying advanced sensors. This study aims to propose a novel hybrid algorithm for endpoint temperature, carbon, and phosphorus based on heat and mass balance and data-driven technique. Three types of static models were established in this study, firstly, theoretical models based on user specified inputs were formulated based on mass and energy balance; secondly, artificial neural networks (ANN) were developed for end-points predictions; finally, the proposed hybrid model was established based upon exchanging outputs and inputs among theoretical models and ANNs. Data of steelmaking production details collected from 28,000 heats from Tata Steel India was used for this article. Model validation was carried out with five-fold cross-validation to ensure generalizations in model predictions.

Oxygen Induced Immiscibility and Ordering in BCC Nb-Ti-Zr Alloys

Michael Waters, David C. Beaudry, Yevgeny R. Shlafstein, Elaf A. Anber, Mitra Taheri, and James M. Rondinelli

(Northwestern University, Johns Hopkins University)

Abstract:

We use the Nb-Ti-Zr composition space to explore how dissolved oxygen

can affect the equilibrium phase diagram and ordering during internal oxidation of multi-principle element alloys. We construct cluster expansion models and machine-learned interatomic potentials as light-weight surrogate models using training data sets of density functional theory calculations. Using Monte Carlo simulations, we compute the effects of oxygen on the equilibrium phase diagram and reproduce experimentally observed microstructures. Furthermore, we perform molecular dynamics starting from our Monte Carlo simulated structures to compare with experimental measurements of short-range order. The Nb-Zr miscibility gap is specifically studied and ternary BCC phase diagrams are reported as a function of dissolved oxygen content.

Dynamic Heterogeneity in Metallic Glass-forming Alloys – A Perspective Form Local Caged Atomic Motion

Hao Zhang

(University of Alberta)

Abstract:

Glass-formation is a ubiquitous phenomenon that is often observed in a broad class of materials ranging from biological matter to commonly encountered synthetic polymer, as well as metallic and inorganic glass-forming (GF) materials. In the supercooled liquids, the dynamics slow down abruptly as the system approaches the glass transition temperature where an enormous change in the rate of structural relaxation is found in association with the growth of string-like collective motion, which could be characterized by "dynamic heterogeneity", i.e., large spatially correlated mobility fluctuations. The Debye-Waller factor (DWF) is the mean square atomic displacement after a fixed decorrelation time characterizing the crossover from ballistic to caged atomic motion, which indicates atomic local mobility in its cage. Recent molecular dynamics simulations of metallic GF systems suggest that the DWF could not only determine the fundamental characteristic temperatures of glass-forming liquids, but only characterize long-time structural relaxation and elastic modulus. In this talk, we will examine how to understand structural relaxation, diffusion, local stiffness, and formation of the shear band during deformation using the DWF in model metallic GF systems.

Computational Fatigue Design of Haynes 282 Alloy Based on Microstructural Deformation Mechanism

Siqi Li

Carleton University

Posters:

A data science-driven approach for structure-porosity linkage of membrane using SEM images

Hooman Chamani

(University of Toronto)

Abstract:

Membranes have achieved a significant place in technology and industry where they are being employed for a broad range of applications, including drug delivery, separation applications, etc. This study integrates the concepts of data science with membrane science with the aim of accelerating the characterization of membranes. In a previous study, 3D structure of a membrane was generated via FIB-SEM. Herein, the 2D images, from the top surface to the bottom surface, were used to create a latent space representation, which could be used as a proxy for detailed explicit quantification of membrane structure. For this purpose, images were segmented and then quantified using spatial correlations. Principal component analysis, which transforms the data coordinates, was used to reduce dimensionality without affecting the useful information embedded in data sets. Afterward, the quantified images were linked to membrane porosity via a regression model. The accuracy of predicted porosity can be proof of the capability of latent space representation for explicit quantification of membrane structure.

Characterization of Zr-Nb-Fe(-Cr) precipitates in Zr-based alloys using density functional theory

Aditya Kamath

(Queen's University)

Abstract:

Zr alloys commonly used in Canada Deuterium Uranium (CANDU) type reactors contain Fe- and Nb-rich precipitates. Some of these precipitates are known to be hexagonal close packed (HCP). In this work, we studied these precipitates using electronic density functional theory, guided by experimental inputs. 122 distinct Zr(Nb,Fe)2, Nb(Zr,Fe)2 and Fe(Zr,Nb)3 compounds were considered. Our calculations suggest that precipitates found in Zr-2.5Nb alloys should be assigned the Zr(Zr,Nb,Fe)2 -- Zr(Zr,Nb,Fe,Cr)2 Laves phase designation. Monte Carlo simulations suggest that these Zr(Zr,Nb,Fe)2 phases are thermodynamically stable at 1073K. Finally, simulated diffraction patterns obtained from ab initio calculated crystal structures match experimental electron diffraction patterns.

Moment tensor potentials from point to extended defects in zirconium

Yu Luo

(Queen's University)

Abstract:

Powerful atomistic-level predictions based on force fields can be fed into predictive models at larger length and time scales (like radiation damage modelling, discrete dislocation dynamics, finite element method). Driven by ab initio or experimental data, A powerful class of machine learning force fields - moment tensor potentials (MTPs) is explored to link highly non-linear association between atomic structures and system energies of zirconium. Numerous MTPs were created and validated. In agreement with ab initio or experimental benchmark, a comprehensive MTP associated with extended defects and point defects in zirconium was proposed in this study.

Computational Material Design for Solid State Batteries

Jacob Rempel

(University of Toronto)

Abstract:

"Solid state electrolyte batteries provide a noticeable advantage over conventional liquid batteries due to their improved safety. In particular, lithium ion solid state batteries have shown exceptional strides in recent years as their cycling performance and electrical capacities have started to approach those of conventional counterparts. In the discovery of these new compounds, Density Functional Theory (DFT) and Ab-Initio Molecular Dynamics (AIMD) are useful tools as they remove the need for a physical laboratory, thus saving time and resources. In addition to this, it has been shown recently that dopants can be used to increase the ionic conductivity of many compounds and this has opened a large field of potential study in doped solid-state electrolytes.

This study takes this computational approach to determine the electronic properties for a variety of compounds, including the Li6PS5X argyrodite series and the Li3SBF4 anti-perovskite series using DFT and AIMD. These compounds have previously been shown to have exceptional long term cycling as well as high discharge capacities. Additionally, they have been experimentally determined to have relatively high ionic conductivities, in the range of mS/cm at room temperature, which has been shown to be linked to improved battery performance. Following this, this study explores the benefits of varying dopants in these compounds and the role they may play in increasing the ionic conductivity of these compounds."

Pixel-embedding U-Net for automatic quantification of microplastic fibres in scanning electron micrographs

Bin Shi

(University of Toronto)

Abstract:

Microplastics becomes a growing threat to the environment and human health. To evaluate the potential risks of microplastic pollution to human beings, microplastics were often examined by visible light microscopy and quantified by labor-intensive visual screening procedures. Among all shapes of microplastics, microplastic fibres, the most abundant pollution in the marine environment, are difficult to count due to their curvilinear and elongated shapes. In our work, deep learning approaches were explored on scanning electron micrographs of fibres collected from daily supplies. U-Net and its variants were used for semantic segmentation and achieved a high average Jaccard index over 0.75. Moreover, pixel-embedding U-Net and TransUNet were implemented for instance segmentation on overlapping fibres. The proposed deep learning approaches facilitated microplastics quantification with high accuracy.

Hybrid Model for Endpoint Prediction in Basic Oxygen Furnace

Ruibin Wang

(University of Toronto)

Abstract:

Strict monitoring and prediction of endpoints in Basic Oxygen Furnace (BOF) is essential for end product quality and overall process efficiency. Existing control models are mostly developed based on thermodynamic principles or by deploying advanced sensors. This study aims to propose a novel hybrid algorithm for endpoint temperature, carbon, and phosphorus based on heat and mass balance and data-driven technique. Three types of static models were established in this study, firstly, theoretical models based on user specified inputs were formulated based on mass and energy balance; secondly, artificial neural networks (ANN) were developed for end-points predictions; finally, the proposed hybrid model was established based upon exchanging outputs and inputs among theoretical models and ANNs. Data of steelmaking production details collected from 28,000 heats from Tata Steel India was used for this article. Model validation was carried out with five-fold cross-validation to ensure generalizations in model predictions.

A Fully Automated Analysis Technique for Electrochemical Impedance Spectroscopy

Runze Zhang

(University of Toronto)

Abstract:

Electrochemical impedance spectroscopy (EIS) is one of the key characterization techniques widely used in diverse fields, such as fuel cells, electrocatalysis and coatings. In EIS a series of small-amplitude electrical perturbations are applied at different frequencies. The resulting impedance response is used to elucidate physical properties such as kinetic rates and processing mechanisms. However, interpreting the EIS data can be quite challenging. EIS spectra are normally analyzed by building equivalent electric circuit models (EECMs). By constructing reasonable EECMs that match experimental data and fitting, the values of different components can be used to calculate the kinetics parameters for the different processes such as charge transfer and interfacial reactions. But generating satisfactory EECMs strongly relies on tacit knowledge, which requires years of experience. It's prone to experiential bias, and "best fit" circuits are often arrived at through trial and error. Worse, EECM uniqueness is not guaranteed even for simple systems. Recent work in the literature has demonstrated automated building and fitting of EECMs via gene expression programming (GEP) and genetic algorithm (GA). However, the non-uniqueness of the solution yields a probabilistic sampling of potential EECMs; meaning for any given iteration of the program a non-physical solution is as likely to be proposed as a non-physical solution. Here we will discuss algorithms for the downselection of potential EECMs through the use of constraint reasoning using both soft human heuristics and advanced electrochemical techniques. The tool being developed provides the expert user with a subset of physically plausible EECMs in the form of EECM diagrams with values for the respective components. The users can then select reasonable models and flag unreasonable models, the latter of which can help train a subsequent machine learning model to penalize such circuits in the future.

Electrochemistry, energy storage and devices

Oral Presentations:

Cold Temperature Performance of Efficient All Solid State Rechargeable Zinc-air Batteries with a Spinel Type MnCo2O4/Carbon Fiber Bifunctional Air Electrode

Zahra Abedi, Dr. Weixing Chen, Dr. Douglas G. Ivey

(University of Alberta)

Abstract:

The cost-effectiveness, safe operation and high energy density of rechargeable zinc-air batteries (ZABs) make them promising candidates for energy storage devices. A ZAB typically contains two electrodes, the air electrode and the metallic zinc electrode, separated by an alkaline electrolyte. The air electrode is usually carbon based. Oxygen reduction and oxygen evolution reactions (OER and OER) occur at the air electrode, both of which suffer from poor kinetics. This affects the efficiency and cycle life of a ZAB.

Using effective electrocatalysts can improve the performance of ZABs. Precious metals, like Pt and Ru, have typically been used as ORR and OER electrocatalysts, respectively. However, these metals are rare and expensive and are not stable during cycling. Alternative electrocatalysts include transition metal oxides (TMOs). Although TMOs are inexpensive, effective and abundant and have high activities towards both ORR and OER, they suffer from poor electrical conductivity. Coupling TMOs with conductive carbonaceous materials can lead to high performance nano-engineered air electrodes with sufficient electrical conductivity.

In this work, spinel type MnCo2O4 was coated on carbon fibers (MnCo2O4/CF), which were utilized to make air electrodes. A polyacrylic acid (PAA)-KOH hydrogel was used as the electrolyte to prepare all solid state ZABs. The battery performance was examined in terms of full cell charge/discharge voltage, power density and cycling life in the temperature range of 25oC to -45oC and was compared with ZABs using air electrodes with the benchmark Pt-RuO2 electrocatalyst. MnCo2O4/CF had superior performance to that of Pt-RuO2 at all temperatures. The efficiencies at 10 mA/cm2 for MnCo2O4/CF and Pt-RuO2 were 63.1% and 61.3%, respectively, at 25oC and 53.0% and 42.8%, respectively, at -10oC. MnCo2O4/CF was able to complete 200 charge/discharge cycles even at -45oC without failing while Pt-RuO2 was unable to complete 200 cycles even at 25oC.

Ni and electric vehicle batteries, an overview

Parvin Adeli

(Nickel Institute)

Abstract:

Electric Vehicle (EV) sales nearly doubled in 2021 as compared to 2020 in North America. In 2022 more than ten million EV sales is expected globally. Batteries are essential to enabling this high EV demand. In this presentation, an overview of the EV batteries with a focus on Ni-based cathode chemistry will be provided. Various aspects of the technology and market developments will be discussed including IP landscape, safety and investments. Furthermore, recent developments with regard to regulations and recycling of these batteries will be presented.

Tuning the interface between anion and cation exchange materials to enhance the energy efficiency of carbon dioxide electrolysers

Tartela Alkayyali, Nana Zhao, David Sinton

(University of Toronto)

Abstract:

The conversion of CO2 to value-added products by electrolysis is an attractive method towards achieving net zero emission goals. However, the current state-of-the-art CO2 electrolysers suffer from high operational costs by consuming electricity required to run the reaction at industrially relevant rates. There is a need to decrease the full-cell voltage to decrease the operational costs - an avenue that is rarely explored in the CO2 electrolysis field. Among the available types of CO2 electrolysers, those employing a bipolar membrane (BPM) in forward-bias mode offer the advantage of reduced CO2 loss to the anode, thereby improving carbon efficiency. Currently, such electrolysers have <13% energy efficiency towards ethylene at 4.0 V and >370 GJ tonne-1 ethylene of energy intensity. In this report, we engineered the interface between the anion exchange membrane (AEM) and cation exchange membrane (CEM), with the aim of reducing the full-cell voltage. Direct membrane deposition (DMD) method was employed to tune the thickness of the membranes to ~12 – 16 μm, which brought about a decrease in the system ohmic resistance as observed through electrochemical impedance spectroscopy, compared to ~193 μm in current BPM electrolysers. The DMD approach was also applicable to other types of CO2 electrolysers, such as AEM electrolysers and CO2-to-CO silver catalyst electrolysers, in both of which we observed reductions in the full-cell voltage. The system performance was furthered improved by investigating various ratios of AEM:CEM materials as well as introducing in-situ membrane treatment. These approaches resulted in >0.9 V reduction in the full-cell voltage at >200 mA/cm2. Overall, this approach is estimated to increase the BPM system energy efficiency to >20% towards ethylene and decrease the overall energy intensity by >100 GJ tonne-1 ethylene, which brings the CO2 electrolysis technology closer to valorization.

Activating the basal plane of two-dimensional transition metal dichalcogenides by alloying for hydrogen evolution reaction

Yiqing Chen, Jun Song

(McGill University)

Abstract:

Two-dimensional transition metal dichalcogenides (2D TMDCs) show promises as highly efficient inexpensive electrocatalysts for hydrogen evolution reaction (HER). However, their performance is extremely limited by the inertness of the basal plane. Combining density functional theory (DFT) calculations and gradient boosting regression, a machine learning workflow has been established to predict the HER activity for a series of 2D cation-mixed TMDC alloys (e.g., Mo(1-x)WxS2, Mo(1-x)WxSe2, Cr(1-x)HfxS2, etc.) of various compositions. It is found that alloying exhibits substantial effect in reducing the Gibbs free energy of hydrogen adsorption (ΔGH) on the basal plane, able to render optimal ΔGH for HER for certain TMDC alloys. More than 15% of the adsorption sites we examined across 38 alloys were identified to be ideal for HER. As a result, we demonstrate that alloying can provide a viable route to activate the basal plane of 2D TMDCs. The mechanism underlying this alloying induced basal plane activation was found to originate from the electronic effect, in particular the p-band shifting, resulted from the chemical composition variation. Our study is expected to serve as a critical step for rational design and exploration of TMDC alloy based catalytic systems.

Development of activated carbon from recycled off-the-road (OTR) mining tires as an anode for Li-ion batteries

Somi Doja, Scott Farnham, Peter Nilsson, Jian Liu, Lukas Bichler

(University of Toronto Institute for Aerospace Studies)

Abstract:

Tires are a vital component of most transportation systems and do not degrade

naturally in the environment. Conventionally, waste tires are discarded in landfills, thus posing severe ecological challenges. Recycling of tires (including mining OTR tires) results in the formation of recovered carbon black (rCB).

In this study, activation experiments were performed on rCB to yield activated carbon (AC) via KOH or CO2 activation. KOH to carbon ratio, temperature, and holding time were varied to study the effect of these parameters on the activation kinetics. A maximum surface area of 994 m2/g was obtained from KOH activation, while 803 m2/g with CO2. The surface area increased with increased activation temperature and time for both agents; however, the micropore volume reduced after a threshold was obtained. Both ACs revealed partial graphitization due to heat treatment. Raman analysis revealed the ID/IG ratio changing from 1.08 to 0.92 and 0.84 for KOH AC and CO2AC, respectively. Both high surface area ACs were tested in Li-ion half cells as anodes. The increased surface area was responsible for an extremely high first cycle discharge capacity of 1853 mAh/g for the KOH-AC cell. However, Li was deposited on the electrode surface with continued cycling, and the irreversible capacity loss was over 40%. The presence of functional groups including OH, C=C, C-H found from FTIR spectroscopy was one reason for irreversible side reactions in the samples resulting in this irreversible capacity drop. Despite the irreversible capacity drop, the stable discharge capacity of the cell was around 600 mAh/g, which was higher than the commercially available graphite anode. Therefore, this study marks a potential use of OTR mining tires in the Li-ion battery industry.

Perovskite catalysts with reduced iridium content for oxygen evolution reaction in corrosive acidic media

Hossein Fadaei, Carl Brown, Georges Houlachi, Houshang Alamdari

(Laval University)

Abstract:

This study we synthesized a series of perovskite-based catalysts for oxygen evolution reactions (OER) in corrosive and acidic environment, such as zinc electrowinning process. The objective was to reduce the content of prohibitively expensive iridium in the benchmark IrO2 catalyst. Br-Ir base perovskite was used as the starting point and the perovskite was doped by other cation elements to achieve BaMxIr1-xO3 perovskite (M stands for cation doping element). The solid-state reaction (SSR) route was used to prepare the catalytic compounds. The crystalline structure and morphology of materials were investigated respectively using XRD and SEM. The performance of the synthesized materials with respect to OER were studied using potentiodynamic polarization and electrochemical galvanostatic tests. The results showed that the catalytic properties of Ir in perovskite structure were significantly improved while the Ir content of the catalysis was substantially lower, compared to IrO2 benchmark. BaNb0.2Ir0.8O3 was the best catalyst among the synthesiized formulations, satisfying the requirements of catalytic activity and longevity. Then, Activated Reactive Synthesis (ARS) was used to further enhance the catalytic performance of the compound. ARS uses a combination of thermal treatment and mechanosynthesis processing to synthesize nanostructured perovskite structure with high specific surface area. ARS resulted in decreasing the crystallite size and increasing the surface area of the catalyst. Its physicochemical properties were characterized using XPS, EDS, TEM, and N2 adsorption-desorption measurements (BET). ARS was shown to be effective methode in in improving the catalytic properties of BaNb0.2Ir0.8O3. Keywords: Perovskite structure, Iridium content, catalytic behavior, optimized catalyst, ARS, benchmark IrO2

Towards High Energy Density in Supercapacitors: Achieving Ideal Pseudocapacitive Behavior with Quantized Capacitance

Yee Wei Foong, Kirk H. Bevan

(McGill University)

Abstract:

Supercapacitors store more energy than double layer capacitors through redox reactions. Ideally, these redox reactions should allow multiple Faradaic electron transfer events that overlap to form a near rectangular voltammetry profile and in this manner mimic double layer capacitance – hence the name "pseudocapacitance". However, current efforts towards achieving this ideal pseudocapacitive behavior via synthesizing complex chemistries can be challenging. In this work, we theoretically demonstrate that quantized capacitance (also known as solvated Coulomb blockade) can serve as viable mechanism to achieve ideal pseudocapacitive energy storage. We analyze the origin of quantized capacitance arising from energy level quantization at the nanoscale. By formulating comprehensive theoretical framework based on electron transfer properties, we are able to explore several factors such as nanoparticle dimensionality and electrolyte dielectric properties; both can be utilized to effectively tune the quantized capacitance behavior and thereby arrive at an ideal pseudocapacitive response. Finally, based on earlier experimental work in the literature, we propose several engineering strategies to experimentally realize quantized capacitance as an energy storage mechanism and optimize its performance towards achieving high energy densities comparable to that of batteries.

Role of planar defects in SOFC electrolytes

Kulbir Ghuman

(Institut national de la recherche scientifique)

Abstract:

The critical challenges related to climate change and energy security could be solved if we can find the champion materials to build sustainable and environment-friendly devices. With this aim in mind, my research leverages leading-edge computational techniques and a multidisciplinary approach to understand the behavior of complex electrolytes currently used in solid oxide fuel cells (SOFCs) and optimize them for next-generation fuel cell devices. The electrolytes used in SOFCs are generally polycrystalline with different grain sizes, grain orientations, dopant segregation, and defects distribution. In addition, they are typically characterized by a high density of grain boundaries and interfaces. All these features can substantially affect their ionic and electronic conductivity. In this talk, I will discuss our recent findings on the microstructural, ionic, and electronic behavior of grain boundaries and interfaces present in commonly used ceramic SOFC electrolytes. By integrating the classical and quantum simulations, this work prepared realistic models of the working-class materials and provided the long-sought explanation for the experimentally observed phenomenon.

Development of self-supported nanostructured multifunctional catalysts for ethanol oxidation

Mohamed Mohamedi

(Institut National de la Recherche Scientifique (INRS))

Abstract:

The direct ethanol fuel cells (DEFCs) are attractive alternative energy sources that may operate at overall net-zero CO2 emissions if bioethanol is used as fuel. Therefore, the development and electrochemical investigation of electrocatalysts for DEFCs are central from both fundamental and practical viewpoints. The usual approach to enhance the performance of Pt towards ethanol oxidation reaction is to incorporate Pt with oxophilic metal oxides (MOx), which can facilitate the

formation of OHad species, for promoting the oxidation of poisoning COad and CHx intermediates (bi-functional mechanism) and Rh for the cleavage of the C-C bond.

In this talk, we focus on our progress in the design and syntheses by pulsed laser deposition technique of free-standing nanostructured ternary anode catalysts Rh-Pt-MO2 (M = Sn, Ce, Mn and Ti) and PtxRh100-x alloys supported either on carbon paper or carbon nanotubes substrates.

To grow high-quality functional thin films at ambient temperature, the pulsed laser deposition (PLD) and cross-beam PLD (CBPLD) techniques were employed.

The surface morphology of the samples was observed with scanning electron microscopy (SEM). The crystalline structure was determined by X-ray diffraction (XRD), whereas X-ray photoelectron spectroscopy (XPS) to assess the surface composition. The catalysts are systematically studied for their tolerance to CO poisoning, their electrocatalytic activity towards ethanol electrooxidation and their long-term durability in acidic electrolyte.

The desolvation and intercalation of Al3+ from Al2Cl7- into a Chevrel phase Mo6S8 cathode in aluminum ion batteries

Jocelyn Riet, Kok Ng, Gisele Azimi

(University of Toronto)

Abstract:

The rapidly growing demand for renewable energy necessitates large-scale energy storage; aluminum ion batteries (AIB) may provide a high performance electrochemical storage method. Aluminum is abundant, has a high theoretical capacity, and is a preferable metal for battery manufacturing while lithium suffers from hazardousness and scarcity. Current work is devoted to understanding how AIBs function under select cathode and electrolyte configurations to design improved AIBs. Our goal is to understand the chemical and/or electrochemical pathway facilitating the intercalation of Al3+ into a Chevrel phase (CP) Mo6S8 cathode, a material unique for that ability.

Characterization of the CP electrode is conducted in conjunction with density functional theory (DFT) calculations. Chevrel phase Mo6S8 is synthesized, characterized, and then implemented into AIBs with an ethyl methyl imidazolium chloride (EMIMCl) / AlCl3 ionic liquid electrolyte. These AIBs are characterized using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and equilibrium polarization curves to reveal information about the intercalation pathway and the cathode's stern layer. The nudged elastic band method (NEB) is used to calculate theoretical energy barriers impeding the desolvation of Al3+ from the ionic liquid.

Synthesized CP cathode that was characterized using x-ray diffraction (XRD) is shown to be of sufficient purity. Separately, bond lengths of all species involved in the desolvation of Al3+ simulated in DFT are within 0.01 Å of values reported in literature. Broadly, it is hypothesized that the intercalation pathway is rate-limited by a reversible chemical reaction that happens before the Faradic charge transfer of Al3+ with Mo6S8; the bond cleavage of Al2Cl7 in the diffusion region is hypothesized to be this reaction.

Multifunctional Materials for Emerging Technologies

Federico Rosei, Daniele Benetti

(Institut National de la Recherche Scientifique INRS)

Abstract:

This presentation focuses on structure property/relationships in advanced materials, emphasizing multifunctional systems that exhibit multiple functionalities. Such systems are then used as building blocks for the fabrication of various emerging technologies. In particular, nanostructured materials synthesized via the bottom–up approach present an opportunity for future generation low cost manufacturing of devices. We focus in particular on recent developments in solar technologies that aim to address the energy challenge, including third generation photovoltaics, solar hydrogen production, luminescent solar concentrators and other optoelectronic devices. [1-23].

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Corrosion and wear of graphene-PMMA nanocomposite coatings made by drop-casting

Amir Reza Salasel, Sukanta Bhowmick, Ahmet T. Alpas

(University of Windsor)

Abstract:

Recent studies have shown that polymer nanocomposite coatings are effective in preventing corrosion. In addition to anti-corrosion properties, polymer matrix nanocomposite coatings should be easy to prepare and possess suitable tribological and mechanical properties. Graphene due to its chemical inertness and high strength has attracted attention as dispersed phase in nanocomposite coatings. In this study, graphene nanoplatelets (GNP) with different weight percentages of 0.5%, 1.0%, and 3.0% were incorporated into poly(methyl methacrylate) (PMMA) using the solution mixing method. Graphene-PMMA coatings were then deposited onto a mild steel surface using a drop-casting method. The structure of GNP sheets with an average diameter of 5μm was characterized using Raman spectroscopy. Scanning electron microscope (SEM) and Raman mapping were employed to investigate the morphology of nanocomposites and the dispersion of GNP in the matrix. GNP sheets were evenly distributed in coatings containing 1.0 wt.% GNP, while overlapping of GNP sheets in the coatings containing 3.0 wt.% GNP was observed. Electrochemical properties of the graphene-PMMA nanocomposites were then evaluated in 5.0 wt.% NaCl solution using potentiodynamic polarization (PDP). The results revealed that, PMMA coatings containing 1.0 wt.% GNP, decreased corrosion rate of the mild steel from 2.6×10^(-1) mmPY to 7×10^(-4) mmPY. Contact angle measurements showed that the 1.0 wt.% GNP nanocomposites indicated a contact angle of 74.12°. The effect of the corrosion on the wear behaviour of the coatings was studied using reciprocating wear test of the coating surfaces after the corrosion tests. In addition, worn coatings are being subjected to PDP tests to investigate the impact of wear on the corrosion of the graphene-PMMA nanocomposites.

Electrodes and Electrolytes Design for Safe and High-Energy Rechargeable Metal-air and Lithium-metal Batteries

Shuhui Sun

(Institut National de la Recherche Scientifique)

Abstract:

"Rechargeable zinc-air batteries (ZABs) and lithium metal batteries (LMBs) are considered among the most promising next-generation energy storage technologies due to their various advantages, such as high energy density.

The Li metal anode is known as the “Holy Grail” electrode for its extremely high theoretical capacity (3860 mAh·g−1). Especially, after pairing with sulfur or oxygen cathodes, ultra-high energy densities above 2000 Wh kg−1 can be obtained, however, serious practical bottlenecks exist. For example, the growth of Li dendrites can generate unreactive Li and even pierce the separator, leading to safety issues. To address these challenges, we developed a simple electrolyte additive strategy to effectively inhibit the growth of Li dendrites, and significantly improve the electrochemical performance of LMBs. For example, the Li|Li symmetric cell exhibits excellent cycling stability above 700 h under a high plating capacity of 3 mAh cm−2. Synchrotron-based X-ray absorption fine structure was used to verify the protective mechanism of additives at the cathode and anode electrodes.[1-2]

The development of highly efficient bifunctional electrocatalysts for oxygen reduction and oxygen evolution reactions (ORR/OER) in ZABs is highly desirable, however, remains a grand challenge. We developed a series of high-performance bifunctional ORR/OER catalysts for rechargeable ZABs systems. The novel nanostructures exhibit excellent energy density and ultra-long cycling lifetime over 1,000 h.[3-12]

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Ta-based Hybrid Catalysts as Non-Noble Metal Catalyst for the Oxygen Reduction Reaction

Ana Tavares, Gaixia Zhang, David Sebastián, Xilin Zhang, Carmelo Lo Vechio, Qilian Wei, Vincenzo Baglio, Weichao Wang, Shuhui Sun, Antonino S. Aricò

(INRS - Centre Énergie Matériaux Télécommunication)

Abstract:

Oxygen reduction reaction (ORR) is a very important process in life and in various energy related applications. In the past decades, the metal oxides of groups 4 and 5 have attracted some interest due to their low cost, abundance, environmental compatibility and excellent stability especially in acid medium [1-3]. However, these transition metal oxides usually exhibit limited catalytic activity and the exact nature of the active sites is not well known. Here, we will present our recent work on Ta-based hybrid catalysts, aiming at the development of Pt-free catalysts with excellent activity for ORR. Among the investigated catalysts, the Na2Ta8O21-x / Ta2O5 / Ta3N5 @ graphene hybrid material has an excellent activity for ORR in alkaline medium and one of the highest reported so far in acid medium [4]. The origin of the catalytic activity for the ORR on these materials will be discussed.

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All-Solid-State Lithium Batteries: from Materials Synthesis to Interface Design to Practical Pouch Cell Engineering

Changhong Wang, Prof. Xueliang (Andy) Sun

(Western University)

Abstract:

All-solid-state lithium batteries (ASSLBs) have gained substantial attention because of their intrinsic safety and high energy density. However, the commercialization of ASSLBs has been stymied by insufficient ionic conductivity of solid-state electrolytes, significant interfacial challenges, as well as the large gap between fundamental research and practical engineering. Over the past several years, we have been dedicated to developing ASSLBs from solid electrolyte synthesis to interface design to engineering practical solid-state pouch cells. First, a wet-chemistry method with a low cost was proposed to produce solid-state electrolytes at the kilogram level with a high room-temperature ionic conductivity (> 1 mS.cm-1). Second, the interfacial challenges of ASSLBs have been well addressed via increasing the ionic conductivity of interfacial buffer layers, manipulating interfacial nanostructures, using single-crystal cathodes,6 deciphering interfacial reaction mechanisms, and constructing artificial solid electrolyte interphases (SEI), which successfully boosted interfacial ion and electron transport kinetics. Resultantly, ASSLBs demonstrated superior electrochemical performance. Third, practical solid-state pouch cells with high energy density have been engineered. Recently, a solvent-free process was proposed to fabricate freestanding and ultrathin inorganic solid electrolyte membranes.10 Furthermore, a feasible solid-liquid transformable interface was devised to improve the solid-solid ionic contact and accommodate the significant volume change of solid-state pouch cells. The resultant solid-state pouch cells successfully demonstrated high energy density and unparalleled safety. In summary, our research not only provides an in-depth understanding of solid electrolyte synthesis and rational interface design but also offers feasible strategies to commercialize ASSLBs with high energy density, low cost, and excellent safety.

Semiconductor assisted photocatalysis for CO2 reduction to liquid solar fuels

Yimin Wu

(University of Waterloo)

Abstract:

Development of sustainable and clean sources of energy, and mitigation of greenhouse gas emissions such as CO2, is among the greatest challenges facing our planet. Recently, electroreduction of CO2 has attracted considerable interest for removal of gaseous CO2. However, it is associated with significant losses primarily due to a large overpotential and electrical energy input. In addition, the use of electricity as a secondary form of energy is inefficient due to significant losses associated with conversion from primary sources to chemical fuels. Solar energy is the largest primary energy source available. Photocatalytic reduction of CO2 using solar energy offers an efficient way to convert solar energy into chemical energy and directly store it in the form of chemical fuels. Particular interest is its conversion directly into liquid fuels such as methanol. We will present CO2 reduction in a metal oxide system, namely Cu2O. It is very promising as photocatalysts with good mutlielectron transfer properties due to its loosely bonded d electrons. It is inexpensive materials with near ideal electronic properties for light energy conversion into fuels. Cu2O shows intrinsic p type conductivity due to presence of negative charged Cu vacancies with one of the lowest electron affinities, identifying Cu2O as an optimal candidate for reduction of CO2. Here, we present atomic level understanding of active sites in Cu2O that leads to the discovery of the facet specific adsorption and subsequent light induced of CO2 exclusively into liquid fuel-methanol. The activity of these active sites was unraveled using operando multimodal correlative scanning fluorescence x-ray microscopy and environmental transmission electron microscopy at atmospheric pressure, in operando, on a single particle level, we design nanoparticles with high active facet selective active sites and particles activity.

Interfacial Solutions for Solid-State Lithium Metal Batteries with Ceramic Electrolytes

Shuo Yan, Ali Merati, Chae-Ho Yim, Elena Baranova, Arnaud Weck, and Yaser Abu-Lebdeh

(University of Ottawa, National Research Council of Canada)

Abstract:

Solid-state lithium metal batteries (SSLMBs) have attracted enormous attention for the application of safe and high-energy storage devices. Among solid-state electrolytes materials applied in SSLMBs ceramics, perovskites (La2/3xLi3xTiO3, LLTO) and garnets (Li7La3Zr2O12, LLZO) are non-flammable, have higher ionic conductivity (>10-4 S/cm at room temperature), and have a wider electrochemical window (>5 V). However, poor contact and chemical instability between ceramics and electrodes have impeded the practical application of SSLMBs.

To investigate the role of different types of interfaces used in ceramic batteries, LLTO pellets were coated with three polyethylene oxide (PEO) based layers: PEO only (P), PEO+salt (PS), and PEO+salt+plasticizer (PLS). Our study showed that the PLS gel membrane reduced the bulk resistance of LLTO down to 84.88 ohm cm-2 and increased ionic conductivity significantly. However, its chemical stability against Li metal was degraded. Compared to PLS membrane, PS layer coated-LLTO sandwiched by Li-metal resulted in the smallest overpotential (1.55 mV at 0.04 mA cm-2) and the assembled cell was stable after 20 cycles without any sign of Li dendrite formation. In addition, a carbonate-based liquid electrolyte (LE) was added at LLZO/NMC 622 cathode interface. The half-cell exhibited an initial discharge capacity of 168 mAh g-1 with a capacity retention ratio of ~82 % after 28 cycles. Scanning Transmission X-ray Microscopy results demonstrated the formation of a robust SLEI (solid-liquid electrolyte interface) during cycling. This SLEI mainly consists of inorganics such as LiF, Li2O, and Li2CO3 that successfully suppressed continuous decomposition of LE and stabilized the performance of LLZO electrolytes.

In summary, it was demonstrated that polymers with salt and plasticizer at the interface effectively reduce the resistance between LLTO and lithium metal. It is believed that further optimization of LE would improve the performance of SSLMBs.

Steric Hindrance- and Work Function-Promoted High Performance for Electrochemical CO Methanation on Antisite Defects of MoS2 and WS2

Xue Yao

(University of Toronto)

Abstract:

CO methanation from electrochemical CO reduction reaction (CORR) is significant for sustainable environment and energy, but electrocatalysts with excellent selectivity and activity are still lacking. Selectivity is sensitive to the structure of active sites, and activity can be tailored by work function. Moreover, intrinsic active sites usually possess relatively high concentration compared to artificial ones. Here, antisite defects MoS2 and WS2, intrinsic atomic defects of MoS2 and WS2 with a transition metal atom substituting a S2 column, are investigated for CORR by density functional theory calculations. The steric hindrance from the special bowl structure of MoS2 and WS2 ensures good selectivity towards CO methanation. Coordination environment variation of the active sites, the under-coordinated Mo or W atoms, effectively lowers the work function, making MoS2 and WS2 highly active for CO methanation with the required potential of -0.47 and -0.49 V vs. reversible hydrogen electrode, respectively. Moreover, high concentration of active sites and minimal structural deformation during the catalytic process of MoS2 and WS2 enhance their attraction for future commercial application.

Simultaneous modulation of selectivity and activity for Electrochemical CO Methanation

Xue Yao

(University of Toronto)

Abstract:

Realizing CO methanation using electrochemical CO reduction reaction (CORR) is crucial for sustainable energy, but catalysts with high selectivity and activity are still required. As known, the structure of active sites can affect the selectivity and the work function of catalysts is useful for modulating the activity. Here we report antisite defects MoS2 and WS2, intrinsic atomic defects of MoS2 and WS2 with a Mo/W substituting a S2 column, as excellent CORR catalysts using the density functional calculations, where the good selectivity is caused by their special bowl structures and the high activity is induced by their low work functions. Moreover, the intrinsic nature of MoS2 and WS2 ensures relatively high concentration, enhancing their attraction for future commercial application.

Low-Pt and Pt-free Catalysts for Hydrogen Fuel Cells

Gaixia Zhang

(Institut National de la Recherche Scientifique)

Abstract:

Hydrogen fuel cells are expected to play a dominant role in future clean energy solutions. However, the use of expensive and rare Pt-based catalysts for oxygen reduction reaction (ORR) at the cathode is one of the main obstacles to the widespread commercialization of hydrogen fuel cells. Therefore, developing highly efficient low-Pt and Pt-free ORR catalysts is one of the key solutions to solve the above-mentioned challenges. INRS team has made major breakthroughs on Fe/N/C catalyst, with the MEA activity and performance approaching that of Pt in fuel cells [1, 2]. However, the durability of all the reported non-noble metal catalysts (including Fe/N/C) is still insufficient for practical applications and its performance decay mechanism is still unclear. We made systematic studies to verify whether iron is at the origin of the first rapid decay (stability problem) of the Fe/N/C catalyst for ORR in PEM fuel cells [3-5]. We further discovered that the pore size near the active FeN4 sites and the hydrophobicity play essential roles in the catalyst stability of Fe/N/C catalysts [6, 7]. Moreover, we also developed other types of Pt-free catalysts for ORR in fuel cells [8-13]. On the other hand, a series of low-Pt catalysts will also be presented [14, 15].

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Posters:

Cold Temperature Performance of Efficient All Solid State Rechargeable Zinc-air Batteries with a Spinel Type MnCo2O4/Carbon Fiber Bifunctional Air Electrode

Zahra Abedi

(University of Alberta)

Abstract:

"The cost-effectiveness, safe operation and high energy density of rechargeable zinc-air batteries (ZABs) make them promising candidates for energy storage devices. A ZAB typically contains two electrodes, the air electrode and the metallic zinc electrode, separated by an alkaline electrolyte. The air electrode is usually carbon based. Oxygen reduction and oxygen evolution reactions (OER and OER) occur at the air electrode, both of which suffer from poor kinetics. This affects the efficiency and cycle life of a ZAB.

Using effective electrocatalysts can improve the performance of ZABs. Precious metals, like Pt and Ru, have typically been used as ORR and OER electrocatalysts, respectively. However, these metals are rare and expensive and are not stable during cycling. Alternative electrocatalysts include transition metal oxides (TMOs). Although TMOs are inexpensive, effective and abundant and have high activities towards both ORR and OER, they suffer from poor electrical conductivity. Coupling TMOs with conductive carbonaceous materials can lead to high performance nano-engineered air electrodes with sufficient electrical conductivity.

In this work, spinel type MnCo2O4 was coated on carbon fibers (MnCo2O4/CF), which were utilized to make air electrodes. A polyacrylic acid (PAA)-KOH hydrogel was used as the electrolyte to prepare all solid state ZABs. The battery performance was examined in terms of full cell charge/discharge voltage, power density and cycling life in the temperature range of 25oC to -45oC and was compared with ZABs using air electrodes with the benchmark Pt-RuO2 electrocatalyst. MnCo2O4/CF had superior performance to that of Pt-RuO2 at all temperatures. The efficiencies at 10 mA/cm2 for MnCo2O4/CF and Pt-RuO2 were 63.1% and 61.3%, respectively, at 25oC and 53.0% and 42.8%, respectively, at -10oC. MnCo2O4/CF was able to complete 200 charge/discharge cycles even at -45oC without failing while Pt-RuO2 was unable to complete 200 cycles even at 25oC."

Effect of End-of-Life (EOL) content in High-Pressure Vacuum-Assisted Die Cast (HPVADC) Aural2 (AlSi10Mg) on corrosion behaviour

Yuki Ando

(McMaster University)

Abstract:

"Cast Al alloys are used in many automotive applications due to their high strength-to-weight ratio with high castability and recyclability. The Al alloy parts that reached their End-of-Life (EOL) are now considered as one of the primary resources to fabricate automotive cast Al alloys, so called secondary Al alloys. The mechanical properties of secondary alloys are at the acceptable range compared to the primary alloy; however, the corrosion behaviour is still not fully understood yet.

In this research, HPVADC Aural2 with different contents (0%, 40%, 75%, and 90%) is subjected to chemical composition and microstructure characterization, as well as various electrochemical characterization techniques. Throughout the chemical compositional analysis with the Inductively Coupled Plasma (ICP) mass spectroscopy, a higher Ti content was detected on the primary alloy while a higher Cu content was observed on the secondary alloys. Microstructure characterization determined that the distribution of Si eutectic and Fe-containing intermetallic particles was different between the primary and secondary alloys. The cyclic polarization measurement demonstrated that the breakdown potential of the primary alloy was the lowest, however, the repassivation potential was the highest. The potential difference between the breakdown potential and repassivation potential of the primary alloy was the smallest, indicating that the repassivation of the meta-stable pits may be facilitated on the primary alloy. The galvanostatic polarization measurements supported the argument with the potential response observed on the primary and secondary alloys. The NaCl-containing agar gel experiment indicated that the primary alloy is the most resistant to localized anodic dissolution.

This research presents the microstructure and electrochemical characteristics of the primary and secondary alloys which are requisite to understand the effect of EOL content used in Aural2 on corrosion behaviour."

Activating the basal plane of two-dimensional transition metal dichalcogenides by alloying for hydrogen evolution reaction

Yiqing Chen

(McGillUniversity)

Abstract:

Two-dimensional transition metal dichalcogenides (2D TMDCs) show promises as highly efficient inexpensive electrocatalysts for hydrogen evolution reaction (HER). However, their performance is extremely limited by the inertness of the basal plane. Combining density functional theory (DFT) calculations and gradient boosting regression, a machine learning workflow has been established to predict the HER activity for a series of 2D cation-mixed TMDC alloys (e.g., Mo(1-x)WxS2, Mo(1-x)WxSe2, Cr(1-x)HfxS2, etc.) of various compositions. It is found that alloying exhibits substantial effect in reducing the Gibbs free energy of hydrogen adsorption (ΔGH) on the basal plane, able to render optimal ΔGH for HER for certain TMDC alloys. More than 15% of the adsorption sites we examined across 38 alloys were identified to be ideal for HER. As a result, we demonstrate that alloying can provide a viable route to activate the basal plane of 2D TMDCs. The mechanism underlying this alloying induced basal plane activation was found to originate from the electronic effect, in particular the p-band shifting, resulted from the chemical composition variation. Our study is expected to serve as a critical step for rational design and exploration of TMDC alloy based catalytic systems.

Unraveling the Origin of Moisture Stability of Halide Solid-State Electrolytes by In situ and Operando Synchrotron X-ray Analytical Techniques

Weihan Li

(University of Western Ontario)

Abstract:

Recently, halide solid-state electrolytes (SSEs) have been reported to exhibit high ionic conductivity and good compatibility with cathode materials. However, the air stability of halide-based electrolytes is one important factor related to ionic conductivity upon exposure to air for practical application. The instability mechanism of Li3InCl6 towards air is not clearly understood. Herein, we for the first time report the application of operando optical microscopy, Raman spectroscopy, synchrotron-based X-ray powder diffraction (SXRD) and in situ X-ray absorption near-edge structure (XANES) for the study of halide electrolyte air stability. Using these methods, we have been able to track the degradation process of Li3InCl6 exposed to air. It is for the first time found that Li3InCl6 is hydrophilic in character, leading to the absorption of moisture from the air and a portion of the Li3InCl6 reacts with the absorbed H2O to form In2O3, LiCl and HCl. Moreover, the remaining electrolyte absorbs H2O to form a hydrate, Li3InCl6·xH2O. The reaction results in a decrease of ionic conductivity. Additionally, the influence of air stability on the practical application of Li3InCl6 has been explored. Li3InCl6 shows much better stability against air with low humidity (3%) and in battery dry rooms, making it a promising SSE for application in commercial lithium-ion manufacturing industry.

Amorphous oxide solid electrolytes via machine learning-assisted high throughput sol-gel synthesis

Valeria Morozova

(University of Toronto)

Abstract:

"Li-ion batteries are approaching their theoretical capacity limits, butting up against performance demands from emergent green technologies. Lithium-metal batteries, which were shelved due to concerns over safety and stability, offer a potential solution. Solid-state electrolytes (SSEs) seek to address Li-metal battery concerns. Unlike liquid electrolytes, SSEs are compact, leak-proof, and impact-resistant. Nevertheless, the sensitivity of structure-property relationships remains a barrier to their development. Studies of large composition spaces are required for optimizing high ionic conductivity, where SSEs currently trail liquid electrolytes by 10-3 S cm-1.

The aim of this work is to screen for high ionic conductivity oxide SSEs by utilizing a combinatorial high throughput approach.

Oxides demonstrate customizability, chemical, and thermal stability. Amorphous oxide electrolytes have a high degree of structural disorder, which promotes fast lithium-ion conduction and eliminates grain boundary resistance. Improvements in ionic conductivity are observed when multiple network formers are utilized. However, optimizing multi-component systems is experimentally daunting. Machine Learning (ML) paired with high-throughput methodology will accelerate discovery of high-performance oxide SSEs.

Binary and ternary combinations of lithium silicate, borate, phosphate, sulphate, and germanate synthesized via sol-gel, will be used to construct initial data sets. Ionic conductivity data will be put through a supervised ML workflow to generate subsequent combinations of higher complexity systems. Promising compositions will be synthesized and characterized by the same combinatorial approach for experimental validation.

The project to-date has focused on high-throughput instrumentation, and synthesizing initial binary composition spaces to optimize combinatorial protocols."

LiNO3 Polyvinyl Neutral pH Alcohol Electrolytes for Solid-State Electrochemical Capacitors

Julian Rosas

(University of Toronto)

Abstract:

Aqueous neutral pH electrolytes have been recently studied to further enhance the energy and power density of electrochemical capacitors (ECs), allowing for safe, light weight devices. Solid polymer electrolytes have been developed to further integrate neutral pH electrolytes for mechanical flexibility and bypass the bulky packaging needed to contain liquid electrolytes. The electrochemical properties of neutral pH electrolytes comprised of polyvinyl alcohol (PVA) and LiNO3 salt were studied and compared with the liquid baselines for ECs. The polymer electrolytes were fabricated with various LiNO3:PVA salt to polymer ratios and monitored for their ionic conductivity, electrolyte film thickness, and water content at ambient conditions. Solid ECs made with bare Ti electrodes achieved a high average ionic conductivity of 20 mS cm-1 after 30 days shelf storage. The ECs were also studied over a temperature range from -40° to 50 °C, for which the 2100:1 and 2500:1 molar ratio electrolytes maintained capacitive profiles and low resistance even at -40°. The performance of solid cells at low temperatures is correlated to the ion hydration and crystal hydrate formation in LiNO3, which was correlated with the shifts of Raman signature peaks, particularly of the deconvoluted HOH stretching band. The temperature dependence of ionic conductivity, and associated changes in activation energy at sub-zero temperatures gives insight into the largely unknown ion conduction mechanism for the LiNO3 system. The understanding of this promising system will aid to enabling safe wide temperature operating, flexible energy storage, and novel form factors to emerging technologies as they become an increasingly important part of everyday modern life.

Corrosion and wear of graphene-PMMA nanocomposite coatings made by drop-casting

Amir Reza Salasel

(University of Windsor)

Abstract:

Recent studies have shown that polymer nanocomposite coatings are effective in preventing corrosion. In addition to anti-corrosion properties, polymer matrix nanocomposite coatings should be easy to prepare and possess suitable tribological and mechanical properties. Graphene due to its chemical inertness and high strength has attracted attention as dispersed phase in nanocomposite coatings. In this study, graphene nanoplatelets (GNP) with different weight percentages of 0.5%, 1.0%, and 3.0% were incorporated into poly(methyl methacrylate) (PMMA) using the solution mixing method. Graphene-PMMA coatings were then deposited onto a mild steel surface using a drop-casting method. The structure of GNP sheets with an average diameter of 5μm was characterized using Raman spectroscopy. Scanning electron microscope (SEM) and Raman mapping were employed to investigate the morphology of nanocomposites and the dispersion of GNP in the matrix. GNP sheets were evenly distributed in coatings containing 1.0 wt.% GNP, while overlapping of GNP sheets in the coatings containing 3.0 wt.% GNP was observed. Electrochemical properties of the graphene-PMMA nanocomposites were then evaluated in 5.0 wt.% NaCl solution using potentiodynamic polarization (PDP). The results revealed that, PMMA coatings containing 1.0 wt.% GNP, decreased corrosion rate of the mild steel from 2.6×10^(-1) mmPY to 7×10^(-4) mmPY. Contact angle measurements showed that the 1.0 wt.% GNP nanocomposites indicated a contact angle of 74.12°. The effect of the corrosion on the wear behaviour of the coatings was studied using reciprocating wear test of the coating surfaces after the corrosion tests. In addition, worn coatings are being subjected to PDP tests to investigate the impact of wear on the corrosion of the graphene-PMMA nanocomposites.

A DFT study of coordination effect on diatom catalysts toward N2 reduction

Xue Yao

(University of Toronto)

Abstract:

As an important raw material of fertilizers and a potential hydrogen energy carrier, the global demand for NH3 is ever-increasing. Now, the industry-scale NH3 synthesis relies on the energy-intensive Haber-Bosch method, and the electrocatalytic N2 reduction reaction (NRR) is regarded as the sustainable alternative due to the mild reaction condition and the renewable energy supply. Diatom catalysts (DACs) attract much interest and could have better performances in catalyzing NRR than single-atom catalysts (SACs). The performances of DACs are highly related to the coordination environment of active diatoms, but the determining role is still unclear. Herein, we use Fe dimer supported on several two-dimensional transition metal dichalcogenides as NRR catalysts and investigate the coordination effect using density functional theory calculations.

Hydrogen steelmaking

Oral Presentations:

Study of Carbon Material Properties formed in Methane Pyrolysis

Mehran Dadsetan, Fawaz Khan, Prof. Erin R. Bobicki, Prof. Murray J. Thomson

(University of Toronto)

Abstract:

Hydrogen is used to produce chemicals and fuels for a wide range of applications. Conventional methods of hydrogen production such as steam reforming and partial oxidation of methane are associated with CO2 production. This study uses microwave-assisted pyrolysis in a bubbling fluidized bed as a novel method to convert methane to solid carbon and hydrogen without forming CO2. The carbon mass balance in this study reveals that gas-phase nucleation during the pyrolysis process is negligible, and the carbon addition mostly happens through the carbon deposition on the surface of initial particles. The surface morphology of the particles is examined using a scanning electron microscope (SEM) which reveals that the pores on the surface of the particles are all covered by the carbon formed in the pyrolysis process resulting to increase in the density of initial particles by 40%. Moreover, as the particles are heated in the reactor, they become highly graphitic. Therefore, X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) techniques are used to investigate the bulk and surface graphitization of the carbon particles. During pyrolysis, pure solid carbon is formed where further modification of it can make this type of carbon suitable for different applications such as steelmaking.

A comprehensive review of hydrogen injection in Blast furnace

Amiy Srivastava, Kinnor Chattopadhyay

(University of Toronto)

Abstract:

Steel industry contributes around 7% of total CO2 emission worldwide. Decarbonization of the steel industry is a game-changing step welcomed by steel producers. Knowledge building on various aspects of hydrogen utilization in metallurgical processes is the key to success in this mission. Blast furnace is one of the prominent sources of CO2 emission in the steel industry owing to its inherent CO-based reduction reactions. Furthermore, total coke rate in a blast furnace is a major contributing factor in the cost of conversion from iron oxides to iron hot metal. Therefore, reduction in carbon input can provide multifold benefits such as reduction in CO2 emission, reduction in total coke rate, etc. The behavior of the furnace varies from plant to plant based on various factors such as input raw material, oxygen enrichment, blast injection flow rate, PCI injection rate, etc. Therefore, modeling the effect of various parameters to evaluate the flow dynamics in different regions of a blast furnace is critical. Previous and ongoing research are extremely helpful to identify initial conditions for these process parameters. Therefore, a detailed technical literature review including modeling strategies, end effects, etc. is presented. This detailed review would help readers to identify the starting point concerning hydrogen injection in their blast furnace.

Top Gas Recycling Revisited to Reduce Blast Furnace CO2 Emissions

Ezra Widajat, Mitren Sukhram, Kyle Lefebvre, Nicholas Aubry, Ian Cameron

(Hatch)

Abstract:

Global steel production accounts for approximately 7% of global greenhouse gas emissions. The sector is dominated by the blast furnace process, which emits 1.5-1.7 t-CO2/t-HM. In response, many new technologies are being investigated to reach net zero carbon emissions, including blast furnace top gas recycling which was found to reduce the carbon rate by 25%. Initially developed as part of the European Community's Ultra Low Carbon Dioxide Steelmaking (ULCOS), Hatch has revisited the concept to assess if hydrogen usage can further reduce CO2 emissions beyond what was originally achieved by the ULCOS team. A two-stage heat and mass balance model of the blast furnace was used to identify viable operating conditions for low carbon operation significantly lower than the published ULCOS trials. The presentation describes the details of the technologies required to use hydrogen to reach the target CO2 emissions.

Carbon Intensity Reduction using Hydrogen in Industrial Furnaces

Chenn Zhou, Tyamo Okosun, Samuel E. Nielson, Armin Silaen Chukwenedum Uzor

(Purdue University Northwest)

Abstract:

Hydrogen use in industrial furnaces has become a popular topic of late, owing to its position as a conceptually simple solution to reducing furnace CO2 emissions. Computational Fluid Dynamics modeling has been employed to study the impacts of hydrogen combustion and reactions in industrial furnaces under a variety of conditions. In the blast furnace, simulations predicted that stable operation could be achieved with up to 30 kg/thm of H2 injection in isolation and up to 15 kg/thm in combination with NG. The expected quenching effects of H2 injection on raceway flame temperature were observed, however, significant CO2 emissions savings were predicted, including a 60 kg/thm reduction in coke consumption for 25 kg/thm of injected H2. In a reheating furnace, scenarios were simulating maintaining the same heat input as a natural gas-fired furnace using hydrogen as fuel. Results revealed a 17% increase in furnace temperature for hydrogen resulting in 6.5% increase in heat flux into the slabs. Similar average thermal stresses were recorded for both cases which was found to be below tensile yield strength acceptable range for AISI type 316 stainless steel (290MPa). Carbon was completely eliminated from the emission gases, but there was 29.88ppm (+124.7%) increase in flue gas moisture concentration. Similar heating conditions were achieved by reducing the total hydrogen fuel flow rate by 18%.

A simple model of nucleation and growth of inclusions during deoxidation and refining of steel

Angshuman Podder

McMaster University

Materials Information and Education

Oral Presentations:

Using Project Based Learning and Modularization of the Materials Science Curriculum to Increase Student Engagement and Improve Learning Outcomes

Liyang Dai-Hattrick
University of Toronto

Abstract:

In the past two and a half years, covid-19 has greatly impacted our lives and education system. Students' achievement of learning outcomes suffered from the disruption of in-person lectures. As educators, this provided us with an opportunity to rethink how we engage and motivate students in their education and redesign the curriculum to help students learn more effectively. Project-base and module-based learnings will be discussed in this talk as the tools that can promote student engagement.

I will first discuss an example of using project-based learning that encourages students to learn by solving real world problems. In the summer of 2020, I redesigned the Intro to Materials Science and Engineering course at the University of Maryland by introducing a semester long project to replace the final exam. The project was integrated with lectures throughout the semester. Students had to apply what they learned in class to choose/propose a state-of-art material for a real-world application. In order to ensure the final result was a team effort, each student had well defined responsibilities which were rotated throughout the semester. As a result of the project, students were observed to be more active participants in discussions with their peers, the TAs, and me. The final reports of this project showed the research during the project deepened students' understanding of the course concepts, in ways that would be challenging to assess with a final exam. Moreover, the projects were filled with enjoyment and creativity. The student feedback and attainment of learning outcomes were very positive and the students were motivated to learn and research contents beyond the textbook.

I will then discuss a proposed reimaging of the UofT MSE curriculum into a module-based curriculum. Here traditional courses are broken down into sub-units that are centered around specific learning objectives. These sub-units form individual units of a concept map that links the learning objectives of each module to the overall curriculum. This approach creates a logical sequence of concepts which build on top of one another while minimizing overlap. The modules break down barriers between the courses and have the goal of allowing students to choose different learning paths to fit better with their backgrounds and needs. The redesigned curriculum would create clear linkages between the learning objectives in an individual course to the critical outcomes of the degree. The modules will be intentionally structured to make explicit how students can reach those outcomes.

Using the prefrontal cortex as a construct for mapping a human-centred materials paradigm

Richard Hibbard
Alberta Health Services

Abstract:

While behavioral and brain scientists are trying to piece together the puzzle of human values, the philosopher Patricia Churchland [1] has proposed that values like safety, human connection, agency, civility, fairness, and openness are embedded in biological matter. The behavioural neuroscientist Joseph LeDoux [2] posits the existence of genetically programmed survival circuits that detect deviations from optimum values of hydration, nutrient depletion, and safety with behavioural dispositions such as seeking water, food, or safety while creating subjective experiences of thirst, hunger, and fear that motivate resolution of the threat. These experiences act as error signals to consciousness of a specific kind of threat. In this presentation LeDoux' theory is expanded to include survival circuits that respond to threats of social isolation, powerlessness, incivility and contamination, unfair obstruction of goals, and deceit with respective subjective experiences of sadness, shame, disgust, anger, and contempt. In response to perceived threats survival circuits activate automatic default behaviours that happen often without full awareness or direct involvement of executive pathways. Most of the time defaults are effective at resolving problems like stopping for a traffic signal. Executive networks in the prefrontal cortex continually monitor the effectiveness of the default, and success promotes learning that strengthens (reinforces) the default and diminishes the error signal. When there is no success the error signal is strengthened, which brings executive pathways online. The executive task is to suppress the default and create and enact new behaviours based on new goals guided by values manifest in emotional experience. Fear creates urges to seek safety, sadness creates urges to seek connection, shame creates urges to stop and reset goals, disgust creates urges to push away, anger creates urges to approach and seek justice, while contempt creates urges to disengage. Since values and their action urges may conflict with each other, there needs to be a hierarchy of responses. Prioritizing values in the order of safety, connection, agency, civility, fairness, and openness optimizes individual mental health and promotes trust and cohesive group functioning. Consequences of new behaviours are appraised for effectiveness in a trial-and-error fashion, and effective behaviours (those that result in diminished error signal strength) are reinforced and with repetition become new defaults.

Defaults arise from basic individual survival imperatives and if unmodified by executive processes tend to be self-focused. Awareness of the minds of others allows for anticipation of what others are likely to do, and this awareness combined with a commitment to applying these values to others is the basis for empathy and group cohesion. Reason alone does not create values, and enactment of a law is a behaviour – a solution to a threat. In summary, in the same way that powered flight without power will succumb to the force of gravity and the fantastically complex material of the body without a constant expenditure of energy will succumb to the forces of entropy, human organizations without values will succumb to the forces of default-driven anarchy and chaos without constant executive attention and commitment to shared values.

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Experiences delivering a 1200 student introductory materials science course remotely using an integrated custom online textbook

Scott Ramsay

University of Toronto

Abstract:

A case study will be presented, describing how the serendipitous pre-pandemic development of an online textbook with integrated videos and questions was successfully used to deliver a fully online course to 1200 students twice during the COVID19 global pandemic. Experiences and insights gathered from this process will be shared.

Portions of the text were written in the years prior to the pandemic to supplement the traditional textbook assigned. Student feedback from these initial sections was positive and so an effort was made to write content for the remainder of the course. Simultaneously, another project was completed to create short 6–10-minute videos covering all the content in the course. These two elements were then brought together in an online textbook and concept checking questions were written and embedded within the text. This online textbook was initially used in parallel with the traditional textbook before replacing the traditional textbook as the assigned text for the course. Student feedback was very positive, commenting particularly on the ease of reading the conversational tone of the text, the engaging and succinct videos. The simplicity of having all the content, including concept checking questions in a single location was also welcomed by the students. In a large, multi-lecture section course the structure of the text also greatly assisted in maintaining consistency across lecture sections.

When COVID19 shut down in person learning it was a surprisingly easy switch to move the entire first year engineering program, for this course, online. Again, student feedback was broadly very positive, commenting on the organization and simplicity of having lectures, text, and questions in a single location. Details will be discussed of the specific way the lectures were filmed that helped to convey the author's personality and promote student engagement. The author intentionally adopted a playful and conversational tone in the textbook. This was somewhat of a gamble initially, however indications are that this style has resonated well with a strong majority of the students.

Some unexpected outcomes have also presented themselves and will be discussed. Additionally, opportunities for future improvements and deployments will be discussed.

Implementation and Evaluation of Gamified Learning Strategies for Level One Materials Science Education

Shayna Earle, Shayna Earle, Liza-Anastasia DiCecco, Dakota M. Binkley, Gerald Tembrevilla, & Bosco Yu

(McMaster University)

Abstract:

Materials science plays a crucial role in early engineering education, where materials selection is critical in design. However, many programs rely on traditional lecture styles to convey fundamental knowledge. While this teaching style is effective, it provides little opportunity to actively engage and expose learners to memorable experiential learning elements. In this work, we introduced a gamified active-learning approach to teach materials science and enhance learner experience in the first-year Integrated Cornerstone Design Projects in Engineering (ENG 1P13) course, connecting theory to practice to demystify the fundamentals. Notably, two types of materials science games were successfully implemented in an adaptable fashion for in-person and virtual teaching styles for over 1000 learners. The first type is adapted based on popular board games, “Materials Battleships” and “Materials Taboo”, where gamified strategies are incorporated to introduce students to materials properties and materials selection. The second involves the design of custom emulators that challenge learners to explore the mechanical and electrical behavior of materials. To evaluate the effectiveness of materials science games, students in the course were surveyed with a university ethics clearance. The results of the survey indicated that over 70% of students found the gamified learning enjoyable. When asked about learning engagement and future stream choices, results showed that students had higher learning engagement and increased interest in materials engineering Moreover, the findings suggested that gamified learning stimulated students’ interest in material science and motivation to participate. Furthermore, students’ anecdotal feedback signified that taking a gamified pedagogical approach in teaching materials science concepts enhanced learning experiences and elevated students' interest in learning fundamental contents critical for their upper-level engineering courses.

Conductive Cotton Fabric Using Laser Pre-Treatment and Electroless Plating

Zuhaib Hassan

(Istanbul Technical University)

Abstract:

This paper presents the fabrication and characterization of laser-treated conductive cotton fabrics by means of copper metallization techniques. The physical properties of the laser-treated knitted samples were examined in terms of thickness, durability, and abrasion impact. Furthermore, the surface topography of the laser-treated substrates was analyzed using a scanning electron microscope (SEM) before and after the coating process and samples demonstrated remarkably uniform deposition of copper metal nanoparticles on the surface of the fabric. An energy dispersing spectroscopy (SEM-EDX) analysis was carried out to determine the elemental composition on the surface of the substrate after the electroless metallization method. The study found that laser-treated samples showed better resistance to wear compared to untreated fabric samples. Since abrasion resistance is key property in electronic textile applications, laser treated samples could, therefore, be ideal candidates for electronic textile applications. As a result, laser treatment has been shown to be successful in improving the abrasion resistance of conductive textile fabrics.

Applying Categories to Materials Models

Kalan Kucera, Glenn Hibbard; John Nychka

(University of Alberta)

Abstract:

The word ‘material’ encompasses an incredible variety of physical systems, ranging across many structures, properties, and behaviours. We recognize this vast array collectively as ‘materials’ while lacking a formal, overarching framework to connect every element of the set of materials. In order to create this framework, we propose the use of Category Theory, a mathematical framework concerned with structures and structuring processes. Through the broad categorization of material models, and the creation of a framework ‘Material Category,’ an encompassing method of connecting models across and between scales of length based on validation of the similarity or equivalence of structures and interactions becomes feasible. Using this methodology, it also becomes possible to begin to construct a verifiable and refinable framework in which to build multi-scalar continuum models for materials systems.

MSE Knowledge Engine

Andrea Mitchell

(University of Toronto)

Abstract:

Materials Science is a rich discipline which compiles extensive information from a wide variety of topics. It is often difficult to convey the details of materials science research in a sufficiently synthesized manner without losing important information, especially when communicated to a broader audience. We are developing strategies to facilitate this communication using the concepts of relationality and categorically structuring information. By shifting the focus to relationality of objects, rather than the objects themselves, viewers can better understand the system as a whole entity instead of a combination of individual components.

The framework we are following uses the idea of a concept map which is a diagram that models concepts, and links them through relationships. A concept map is created by a diagram which has concepts written in boxes, and arrows connecting each concept. Specifically, we are connecting this idea with Category Theory, which is a branch of mathematics which studies the relationships between mathematical structures. In applying this to science, mathematician David Spivak created a model he calls an “ontology log”, commonly abbreviated “olog”. In this way, we can analyze the similarity between concept maps both by the similarity of the topic, as well as the similarity in the structure of the map. From the perspective of MSE, we are creating frameworks to structure information in the form of material categories, which allows for the exploration of materials through different contexts.

Long term goals of the project include creating an online database of current research in the MSE department in the format of concept maps. Additionally, this framework will be used to create a database of MSE undergraduate content, which will act as a tool for education for undergraduate students in the department.

Design And Analysis Of A Rear Bumper Of An Automobile With A Hybrid Polymer Composite Of Opebf/Banana Fibres

Solomon Ochuko Ologe, Duru C.A, Anaidhuno U.P

(University Polytechnic Of Catalonia, Barcelona)

Abstract:

This research investigated the design and analysis of a rear bumper of an automobile with hybrid polymer composite of OPEBF/Banana fibre . OPEBF/Banana fibre hybrid polymers composite are of low cost, light weight, as well as possess satisfactory mechanical properties. In this research work, hybrid composites have been developed using hand layup technique based on percentage combination of OPEBF/Banana fibre at 10:90, 20:80, 30:70, 40:60, 50:50. 60:40, 70:30. 20:80, 90:10, 95:5.. The mechanical properties in the context of compressive strength of 65MPa, flexural strength of 20MPa and impact strength of 3.25Joule was observed and the simulation analysis on the induction of 500N load at factor of safety of 3 were observed to have display a good strength suitable for automobile bumper with the advantages of weight reduction.

Connections in Training

Chloe Shao, Carson Dueck, Danica Drago

(University of Toronto)

Abstract:

Training converts observations to knowledge, knowledge to understanding, understanding to decisions, and decisions to actions. We see a system, consider our observations, use those observations to define a path forward, and implement that path forward. Training is often focused on the use of specific tools; they may be thinking tools, communication tools, or physical equipment. This training is present in any problem-solving based field that requires adaptive approaches. In this presentation, we will focus on artists, pilots, and engineers. Artists, pilots, and engineers must be capable of working through challenges we have not been explicitly trained to deal with. For example, an artist may be faced with a new medium, a pilot may be faced with a new destination, and an engineer may be faced with a new client's particular requirements. These may seem distinct, but the human brain addresses them in precisely the same way. First, it will try to apply already known strategies to these new circumstances. If this works, the use of these strategies for these circumstances will be reinforced. If it does not work, the prefrontal cortex activates to create a new strategy while suppressing the default/trained strategy. The new strategy will be applied, evaluated, and iterated on if necessary. Effective training facilitates this adaptive approach because it creates proficiency without creating dependence. Proficiency is the expert-level use of knowledge while dependence can lead to overuse/inappropriate use of a specific lesson where it likely does not apply. In this presentation, we will abstract and compare the training strategies used to create the proficiencies represented in the three presenters, along with a generalized approach to teaching/training that can be used in each of our fields.

Practical Colorimetry for Scientific Visualization

Michael Waters

(Northwestern University)

Abstract:

From simple plots to cutting-edge virtual reality systems, every field of science, technology, engineering, and medicine uses color in their data visualizations. Despite human color perception being an active area of research, aesthetics drives most color choices. Using uniform color spaces derived from models of human color perception, color choices can be designed. Thus, the practical goals for this talk are: (1) to introduce researchers in any field to colorimetry, (2) to give an intuitive understanding of human color perception for data visualization, and (3) to demonstrate the use of uniform color spaces for high-fidelity color choices in data visualization.

The introduction connects the basic physics of sight to color perception on displays by covering the basics of human vision, tristimulus, chromaticity coordinates, and the sRGB gamut. From there, perceptually uniform color spaces are introduced and applied in order of increasing nuance to: improving color choices, color mapping/heat maps, phase-amplitude mapping, chemical mapping, and representations of the visible spectrum. Colorblindness is discussed, including approaches for accommodation.

Posters:

Development of Flexible Humidity Sensors Based on the Corrosion and Degradation of Conductive Substrates

Aleisha Cerny

(University of Toronto)

Abstract:

Water and moisture sensing has become an increasingly essential feature measured in clean energy and transportation applications such as in hydrogen fuel cell vehicles (HFCV). HFCVs are at the forefront of replacing conventional gasoline engines and phasing out the use of fossil fuels in the automotive sector, combatting the urgency of Climate Change. In this study, we develop novel sensors able to detect humidity through two distinct conductive technologies (1) through a change in morphology using conductive water-soluble polymer composite foams and (2) through a rust-induced change or a resistance change caused by the corrosion of a metal substrate. The conductive foam composites will enact a large morphological change and resistance change. The onset of moisture will collapse the microstructure cells, degrading the conductive network, causing a permanent structural change and electrical disconnect able to be detected by an external reader. Five different foam sensors were successfully fabricated, tested, and were determined as functional humidity sensors following their moisture response with time. The foam morphologies were characterized by scanning electron microscopy (SEM), the thermal properties were characterized using differential scanning calorimeter (DSC) and thermogravimetric analysis (TGA) and finally the mechanical properties were measured using dynamic mechanical analysis (DMA). The second sensing technology encompasses a magnesium-copper galvanic system that when in contact with water for extended periods of time, will corrode (i.e., convert the metal into metal oxide) causing an irreversible change through an increase in resistance, subsequently alerting the user of possible water flooding. The metallic sensors were tested at various outdoor temperatures (0°C, 23°C and 50°C) in order characterize the influence of temperature by measuring the resistance increase with time. They were also tested with a direct force where the corrosion was accelerated.

Nuclear energy materials and environmental degradation

Oral Presentations:

The role of carbide precipitates in hydrogen embrittlement of high strength steels

Xiaohan Bie

McGill University

Abstract:

Carbide precipitates play an essential role in both strengthening and mitigating hydrogen embrittlement (HE) susceptibility of steels. In particular, vanadium and niobium carbide precipitates in steels provide irreversible traps for hydrogen atoms, significantly reducing steels' HE susceptibility. Carbon vacancies in precipitated carbides offer numerous strong H traps. However, systematic characterizations of the exact H trapping sites and strengths of those carbide precipitates are absent. In the present work, systematic first-principles calculations were performed to determine the ground state structures and mixing energies of vanadium and niobium carbides as the carbon content varies. Different vacancy patterns were identified, which were found to be dominated by the mechanical interaction between vacancies. These vacancy patterns were found to have significant influence of hydrogen trapping energies and diffusion barriers. Our findings provide valuable insights towards quantifying the effect of sub-stoichiometric carbides on hydrogen trapping and kinetics.

He bubble growth in Ni using object kinetic Monte Carlo

Keyvan Ferasat

Queen's University

Abstract:

Helium can be formed in Ni and Ni-based alloys due to (n,α) transmutation reaction. The existence of He leads to nucleation and stabilization of cavities, which may cause catastrophic failure of the nuclear structural components. Being a noble gas, helium is trapped in regions with excess volume such as dislocations, grain boundaries, vacancy, and vacancy clusters. Temperature and damage rate can affect the size distribution of defects as well as cavities and bubbles. Object kinetic Monte Carlo (okMC) is a meso-scale simulation technique. It can capture void evolution. Here, modular Monte Carlo (MMonCa) simulator is used to run okMC simulations. OkMC needs a thorough database of formation, binding, and migration energies as well as dissociation rates to simulate bubble evolution. Our simulations indicate that the bubble size correlated with temperature and inversely dependent on damage rate. Moreover, the bubble size distribution indicates good agreements with experimental studies. We showed the capability of okMC as a tool to study He bubbles formation and growth in pure Ni as a model for Ni-based alloys.

Thermal Aging of Fire-Protective Fabrics used in the Outer Shell of Firefighters' Protective Clothing

Md. Saiful Hoque, Patricia I. Dolez

University of Alberta

Abstract:

Fire-protective fabrics made from high-performance fibers are used to manufacture protective clothing for firefighters, oil and gas industry workers, electricians, and defense personnel, for instance. Apart from protecting the wearer from various hazardous conditions, these fire-protective fabrics must retain their protective performance over time while exposed to various damaging conditions such as heat, ultraviolet (UV) radiation, moisture, and maintenance. Among these damaging conditions, prolonged thermal exposure can cause the fabrics' premature aging, eventually leading to compromised protective performance. To better understand the effect of thermal aging conditions on the long-term performance of fire-protective fabrics, this study exposed three fabrics corresponding to typical blends used as outer shells in firefighters' protective clothing to temperatures between 150°C to 320°C for up to 1200 hours. After exposure to thermal aging, all three fabrics exhibited a significant loss in tensile strength even when accelerated aging was performed at 190°C, which is equal to or below the continuous operating temperature of the high-performance fibers used to manufacture these fabrics. Furthermore, the morphological analysis of unaged and aged fabrics revealed the breakage of fibers due to aging, which can be associated with the reduction in tensile strength of the fabrics observed after thermal aging. Exposure to thermal aging also caused the deterioration of the fabrics' water repellent finishes as shown by changes in the water contact angle of the aged fabric specimens. At the most severe thermal aging conditions, chemical changes were also recorded by ATR-FTIR analysis. The study provides an insight into the aging behavior of high-performance fabrics used in protective clothing against heat and flame. The results obtained can also be used to support the development of end-of-life sensors and predictive models of the aging of fire-resistant fabrics.

A parametric study of crack nucleation and propagation in Zr single crystals

Saiedeh Sadat Marashi, Hamidreza Abdolvand

Western University

Abstract:

A crystal plasticity finite element model is used to study the evolution of cracks in a notched zirconium single crystals. The hexagonal close-packed (HCP) crystal structure with a high degree of elastic and plastic anisotropy is used in simulations. Four different damage initiation criteria are considered, namely the maximum principal stress, the maximum shear on the most activated slip plane, the maximum principal plastic strain, and the maximum energy stored in dislocations. Attention is given to the influence of the effective displacement, crystal orientation, and failure parameters on the stable crack growth and crack growth velocity. It is shown that by decreasing the effective displacement of the crack evolution law, the crack growth rate decreases for all damage criteria. In addition, by increasing the misorientation between the loading direction and the HCP crystals c-axis, the crack velocity increases in all damage criteria except for the maximum principal stress method in which the crack velocity decreases.

Influence of Thermal Aging on the Strength of Moisture Barriers used in Firefighters' Protective Clothing

Laura Munevar-Ortiz, Dr. Patricia I. Dolez and Dr. John A. Nychka

University of Alberta

Abstract:

The moisture barrier is an essential layer in firefighters' protective clothing because it prevents water entry while allowing the body perspiration to exit. Over time the performance of the moisture barrier degrades because of exposure to the different conditions to which firefighters are exposed in service, including high temperatures. Researchers have shown that the most critical layer in the protective clothing when investigating thermal aging is the moisture barrier since it can easily be damaged by heat and may lose its breathability, thus creating vulnerabilities to severe burns. This study aims at examining the effect of thermal aging on the tear strength of moisture barriers. Three moisture barriers used in firefighters' protective clothing were selected for the study. The accelerated thermal aging was carried out in an electric convection oven. Specimens were subjected to aging at 190, 220, and 235 or 240°C (depending on the moisture barrier). The aging times range from 1 to 1056 h. The aging temperatures were selected considering the conditions faced by firefighters. The residual tear strength of the fabrics was measured by the trapezoidal procedure following the ASTM D5587-15 standard test method; however, due to limitations in fabric availability a slightly smaller specimen size (55 x 110 mm) was used. One-way analyses of variance were carried out to analyze the influence of the aging time and temperature on the mean tear strength. Scanning electron microscopy was used to evidence any potential changes in the surface due to thermal aging. The results obtained show that thermal aging at temperatures of 190°C and higher reduce the tear strength of the moisture barriers tested more than 50% at the longest aging time. In addition, two of the moisture barriers showed shrinkage, cracks, and delamination when exposed to 240°C or higher. These preliminary results demonstrate the importance of better characterizing and understanding the effect of thermal aging.

High-Resolution Characterization of The Cyclic Oxidation Behaviour of Fecral Alloys In Steams

Victor Okoro, Kevin Daub, Heidi Nordin, Suraj Persaud

Queen's University

Abstract:

Accident tolerant fuels (ATF) cladding that possesses good oxidation resistance during critical accident scenarios is valuable for the sustainability and safety of light water reactors. FeCrAl alloys possess high-temperature oxidation resistance ability due to the alumina scale formation on the alloy surface, making them attractive candidate material for the ATF cladding in nuclear power plants. FeCrAl alloys were thermally cycled in steam, and preliminary analysis using SEM/EDX shows the predominance of Al2O3 on the interface and mixed oxide around the oxide penetration regions dependent on the microstructure of the alloys. All exposure conditions showed outward diffusion of Al to the surface, forming a protective solid-state diffusion barrier reducing the reaction between the alloy and the surrounding environment. The results reveal the predominance of Al2O3 and Fe-rich metal zones at areas where oxide penetrations are present in the interface.

Furthermore, advanced transmission electron microscopy techniques were used to investigate the cyclic oxidation behaviour of FeCrAl alloys exposed to a pure argon/steam environment at 1000°C. Using the steam rig and high-resolution imaging (TEM/EDX, EBSD), oxide penetrations on the FeCrAl alloys were characterized at the nanoscale. The high-resolution imaging intended to be performed will reveal the grain orientation that forms the outward growing alumina scales highly susceptible to oxidation. The results further support the use of this alloy as an ATF cladding material.

Hydrogen clustering in bcc metals: stress anisotropy, junction function and damage accumulation

Jun Song, Jie Hou

McGill University

Abstract:

Hydrogen (H) is known to induce damages in metals and post great threat to relevant applications. These damages usually involve H concentrated in a local region, one form of which is H clustering. However, the feasibility and atomic origin underlying H clustering remains contended, particularly for non-hydride forming metals. In our work, based on ab initio and atomistic modelling, we systematically investigated H clustering behavior in bcc metals. We explicitly show that H clustering is energetically favorable due to long-ranged elastic H-H attraction and can be strongly facilitated by anisotropic stress field along particular crystalline directions. A linear elasticity model was established to elucidate the origin of the anisotropy and provide predictions for H clustering under arbitrary stress states. We further demonstrated that platelet-shaped H cluster formation is thermodynamically possible at relatively low H concentrations around certain dislocations. Such H clustering can further promote the formation of dislocation junctions which are otherwise unstable in absence of H. The H clustering enabled dislocation junctions can stay stable under shear loading, subsequently promote vacancy loop formation and accumulation, a necessary precursor for H-induced damages such as blistering and cracking. Close agreement between our findings and recent experimental observations has been demonstrated. The present study provides critical mechanistic understanding of H clustering and associated damages in metals.

Statistical distribution of spontaneous recombination radii of Frenkel pairs in FCC and BCC metals

Hao Sun, Laurent Karim Béland

Queen's University at Kingston

Abstract:

The recombination radius of Frenkel pairs generated by incident high-energy particles represents a critical determinant of irradiation-induced microstructure evolution. Mesoscale models of radiation damage evolution that include recombination radii as input parameters can benefit from a better understanding of the atomistic processes controlling recombination. This work used the kinetic activation relaxation technique—an off-lattice, self-learning kinetic Monte Carlo algorithm in conjunction with molecular dynamics simulations—to study the statistical distribution of the recombination radii in six FCC (nickel, copper, silver, gold, palladium, and platinum) and one BCC (iron) structures. We found that recombination can occur from the 2nd nearest neighbor site (neighbor site) to as far as the 15th neighbor site. Long-range recombination is realized via crowdion formation. Vacancies were found to have no effect on interstitial migration, aside from diminishing the recombination energy barriers, which are linearly related to diffusion energy barriers. No correlation was found between energy barriers and the average recombination radii. Instead, the average recombination radius was found to increase linearly with the elastic constants of FCC metals. The atomic displacement field near self-interstitials was found to be identical in different metals. However, metals with higher elastic constants exhibit larger local stresses and broader stress distribution, facilitating long-range recombination. Similarly, hydrostatic pressure enhances the average recombination radius by rising elastic constants. Thus, the elastic constants of FCC metals determine the average recombination radius, not energy barriers.

Hydrogen diffusion towards notch tips in zirconium alloys

Alireza Tondro, Hamidreza Abdolvand

Western University

Abstract:

Hydrogen embrittlement is an important degradation mechanism affecting the lifetime of engineering components. The diffusion of hydrogen atoms into the metal lattice can be affected by the localized stresses that develop around service-induced flaws. Microstructural effects can be significant, particularly in metals such as zirconium with a high degree of elastic and plastic anisotropy. This study uses a coupled diffusion-crystal plasticity finite element approach to quantify the contribution of texture and microstructure to the hydrogen diffusion towards microscale notches. The results indicate that material texture can significantly affect the distribution of hydrogen atoms, the location of maximum hydrostatic stress, and the location of maximum hydrogen concentration. It is shown that as the notch tip becomes sharper, the contribution of texture in determining hydrogen localization becomes less significant.

Ultrafine-grained and nanocrystalline austenitic or ferritic steels for nuclear applications

Haiming Wen

Missouri University of Science and Technology, USA

Abstract:

Bulk ultrafine-grained and nanocrystalline metals possess drastically higher strength than their conventional coarse-grained counterparts, and are anticipated to have significantly enhanced irradiation tolerance owing to the role of grain boundaries as sinks for irradiation-induced defects. In this study, ultrafine-grained and nanocrystalline austenitic or ferritic steels were manufactured by equal-channel angular pressing (ECAP) and high-pressure torsion (HPT), respectively. The microstructure and mechanical behavior of these steels were carefully studied, indicating significantly improved hardness/strength in ultrafine-grained and nanocrystalline steels. The thermal stability of the ultrafine-grained and nanocrystalline steels was also investigated, indicating good thermal stability up to ~600 oC. For ferritic FeCrAl alloys with different ranges of grain sizes, thermal aging was conducted to study thermally induced α' Cr precipitation, which typically cause embrittlement. Results indicated that with decreasing grain size, thermally induced α' Cr precipitation was reduced. Ion irradiations were performed to study irradiation behavior. The ultrafine-grained and nanocrystalline austenitic 304 steel manufactured by ECAP and HPT possess enhanced phase stability during irradiation, compared to their coarse-grained counterparts. Smaller grains possess reduced irradiation-induced hardening, segregation and precipitation compared to larger grains. In ion irradiated ferritic FeCrAl alloys, it was also found that a reduction in grain size led to reduced irradiation-enhanced α' precipitation, and that in nanocrystalline FeCrAl alloy, there was no α' precipitation after irradiation. All these results indicate enhanced irradiation resistance of ultrafine-grained and nanocrystalline steels and their great potential for nuclear applications.

Oxidation of Silicon Carbide and Graphitic Materials of TRISO Nuclear Fuel in Oxygen Containing Environments

Haiming Wen, Adam Bratten, Visharad Jalan

Missouri University of Science and Technology, USA

Abstract:

While high-temperature gas reactors use pure helium as a reactor coolant, in some accident scenarios significant amounts of air can be introduced, resulting in varying oxygen partial pressure. It is important to understand the oxidation processes exhibited by both TRISO particles (particularly the SiC layer) and matrix graphite under these conditions. The TRISO particles are bonded using graphitic matrix materials into a cylindrical fuel compact or spherical pebble. Matrix-grade graphite is graphitic material composed of multiple types of graphite and carbonized phenolic resin. In this study, matrix graphite and surrogate TRISO particles were subjected to oxidation at temperatures ranging from 1000 to 1600 oC in environments containing different partial pressures of oxygen, using box furnace or thermogravimetric analysis – differential scanning calorimetry. The microstructures of the materials before and after oxidation were carefully characterized via different techniques. The thickness of the oxide scale on SiC at different temperatures with different partial pressure of oxygen was quantitatively measured, and the rate constants and activation energy for oxidation were determined accordingly. The oxidation mechanisms were ascertained in relation to the oxidation conditions and microstructures of the materials. Results indicated that differences in the oxidation rate and behavior between different grades of matrix graphite are caused by the microstructural differences and the difference in partially graphitized carbon content. Oxidation of SiC in 20 kPa oxygen can be effectively described as passive oxidation, producing oxide scales with uniform thickness. Oxidation of SiC in 0.2 kPa O2 produces nonuniform oxide layer. Protruding nodules, inside which pores and cracks exist, were identified on the oxide surface under which ultrafine-grained SiC grains were present. Such nodules are attributed to active oxidation followed by redeposition of crystalline SiO2.

A Mesoscale Model of Dry and Hydrated Montmorillonite

Yaoting Zhang, W.J. Binns, S.Briggs, C.K. Kim, L.K. Beland

Queen's University

Abstract:

Bentonite is one of the barriers in deep geological nuclear waste repositories. Montmorillonite (MMT) is the main mineral component of bentonite. In the presence of water, MMT swells and reduces water flow, which makes it a great corrosion prevention barrier.

A number of atom-scale computer-based simulations of MMT are able to capture this swelling phenomenon. Notably, all-atom molecular dynamics can capture important structural properties of MMT such as its hexagonal shape, proper strength of sodium interaction with oxide chains and flexible hydroxyl edges. However, all-atom molecular models are computationally expensive and do not handle enough atoms to be compared with experimental results. In this work, we present two coarse-grained models of MMT: dry and hydrated MMT. Having systems at both hydration extremes allows us to study systems at different humidity levels. Each MMT platelet was divided into central non-bonding and edge hydrogen-bonding particles. The coarse-grained particles interact through pair interactions. The pair potential parameters were optimised based on potentials of the mean force between two MMT platelets with radius of 12 Å in various configurations obtained by all-atom molecular dynamics simulations. The mesoscale model is used to simulate systems larger than those accessible to all-atom molecular dynamics. We present a hydrated MMT system composed of 1000 platelets each with a radius of 60 Å, and compare their Young's and shear moduli to experimental values. In the future, we plan to use this model to investigate the pore network of MMT and establish a connection with existing continuum models.

Posters:

The study of one-dimensional gliding defect clusters in zirconium using numerical simulations

Amir Ghorbani, L.K. Beland

Queen's Uinversity

Abstract:

Neutron-irradiated Zr undergoes directional growth and creep, which can be an issue during operation of CANDU reactors, as Zr alloys are used as fuel channel structural materials. This directional growth and creep is generally thought to be associated to anisotropic transport of irradiation-induced defects in the Zr crystal structure. Here, we perform molecular dynamics simulations to study self-interstitial defect clusters created by high-energy collision cascades induced by neutron-Zr interactions. We first re-parametrize a model to describe interatomic interaction forces, combining the so-called embedded atom model (EAM) to electronic density functional theory (DFT) calculations. Second, we simulated 64 high-energy collision cascades using molecular dynamics and this newly reparametrized interaction potential. Finally, we analyzed the radiation-induced point defects and defect clusters. Notably, we identified self-interstitial clusters that diffuse in one dimension along prismatic crystal directions; such one-dimensional diffusion will lead to important anisotropy of diffusion.

Modelling of the interaction and reorientation of zirconium hydrides

Alireza Tondro, Brooke Bidyk, Ivan Ho, Kian Khaksar, Hamidreza Abdolvand

Western University

Abstract:

Hydrogen embrittlement is one of the major concerns in nuclear industry. Formation of zirconium hydrides significantly accelerates the degradation of zirconium alloys used in the core of nuclear reactors. Zirconium hydrides usually form in different directions and configurations. This work studies the developed stress fields due to the interaction of hydrides and their subsequent effects on redistribution of hydrogen atoms. The effects of hydride distance for different hydride configurations are investigated in a CANDU pressure tube using a coupled diffusion-crystal plasticity finite element approach. It is shown that, due to alignment of growth directions of hydrides, stress fields in the vicinity of two parallel hydrides interact more significantly compared to those of perpendicular hydrides. Also, the effects of hydride length and width are studied where it is shown that hydrides with a width of 1 um propagate faster than those having lower and higher widths.

Microstructural Comparison of Pyrophosphate and Acid Copper Coatings for Canada's Used Nuclear Fuel Containers

Sang Bum Yi, Jason Tam, Jason D. Giallonardo, Jane Y. Howe, Uwe Erb

University of Toronto

Abstract:

The Nuclear Waste Management Organization (NWMO) is developing a deep geological repository (DGR) for the permanent disposal of Canada's used nuclear fuel. The DGR employs an engineered barrier system (EBS) to contain and isolate used nuclear fuel from the environment. A key engineered component of the EBS is the used fuel container (UFC). The UFC is the vessel in which used fuel is packaged. It consists of a carbon steel structural vessel with a minimum 3 mm copper coating bonded to the external surface for corrosion protection. The UFC components (upper hemi-head and lower assembly) are copper coated in a factory setting via an electrodeposition process using either a pyrophosphate-based electrolyte or acid-based electrolyte. The corrosion behaviour of the copper coating may vary depending on its microstructure, which is influenced by the synthesis process and conditions. In this study, thorough microstructural characterizations using electron backscattered diffraction (EBSD) were performed on the electrodeposited copper coatings made by the two different electrolytes. Grain size, grain morphology, crystallographic texture, and grain boundary characteristics were analyzed to develop a better understanding of the synthesis-structure-property relationships. The findings of the present work will support NWMO's ongoing research activities concerning corrosion and mechanical behaviour of the electrodeposited Cu coatings.

Oxidation of Silicon Carbide and Graphitic Materials of TRISO Nuclear Fuel in Oxygen Containing Environments

Haiming Wen, Adam Bratten, Visharad Jalan

Missouri University of Science and Technology

Abstract:

While high-temperature gas reactors use pure helium as a reactor coolant, in some accident scenarios significant amounts of air can be introduced, resulting in varying oxygen partial pressure. It is important to understand the oxidation processes exhibited by both TRISO particles (particularly the SiC layer) and matrix graphite under these conditions. The TRISO particles are bonded using graphitic matrix materials into a cylindrical fuel compact or spherical pebble. Matrix-grade graphite is graphitic material composed of multiple types of graphite and carbonized phenolic resin. In this study, matrix graphite and surrogate TRISO particles were subjected to oxidation at temperatures ranging from 1000 to 1600 oC in environments containing different partial pressures of oxygen, using box furnace or thermogravimetric analysis – differential scanning calorimetry. The microstructures of the materials before and after oxidation were carefully characterized via different techniques. The thickness of the oxide scale on SiC at different temperatures with different partial pressure of oxygen was quantitatively measured, and the rate constants and activation energy for oxidation were determined accordingly. The oxidation mechanisms were ascertained in relation to the oxidation conditions and microstructures of the materials. Results indicated that differences in the oxidation rate and behavior between different grades of matrix graphite are caused by the microstructural differences and the difference in partially graphitized carbon content. Oxidation of SiC in 20 kPa oxygen can be effectively described as passive oxidation, producing oxide scales with uniform thickness. Oxidation of SiC in 0.2 kPa O2 produces nonuniform oxide layer. Protruding nodules, inside which pores and cracks exist, were identified on the oxide surface under which ultrafine-grained SiC grains were present. Such nodules are attributed to active oxidation followed by redeposition of crystalline SiO2.

A hybrid rate theory model for analysis of radiation-induced growth

Mahdi Mohsini, Peyman Saidi, Mark R. Daymond

Department of Mechanical and Materials Engineering, Queen's University

Abstract:

Difference in the diffusivity of radiation products in <a> and <c> directions of Zr unit cell results in phenomena such as irradiation-induced growth and creep. One classical approach to explain this phenomenon is via Diffusional Anisotropy Difference (DAD), which suggests dissimilar rates of diffusion for individual vacancies and interstitials in basal and prismatic planes. An alternative mechanism, known as self-interstitial cluster diffusion (SICD), relates growth to the formation of selfinterstitial clusters which diffuse solely along the <a> axis.

Both DAD and SICD models have limits, with inaccuracies when compared to real experimental data. For example in DAD the ratio of diffusion coefficient of interstitials and vacancies in the <a>-direction and <c>-direction of Zr should be between 3-4 based on ab initio models, but need to be 102 for DAD to give good agreement with experiment. For SICD only dislocation loops are considered, while the influence of other substantial sinks in the material need to be addressed. We propose a hybrid model, in which both aforementioned limitations have been addressed. This makes the hybrid model generalizable and provides good agreement with experimental data while maintain input parameters within physically reasonable bounds. In this model, the combination of point defects and SIA clusters exist and diffuse to the sinks in the bulk and dislocation loops in the prism planes respectively. Furthermore, the bias factor was considered for the cases of polycrystals and cold worked polycrystals to expand the generalizability of the model. Consequently, the sinks of grain boundaries and the enhanced dislocation density due to cold work were captured.

Physical metallurgy and nanomaterials

Oral Presentations:

Highly Ordered Arrays of Gold Nanorings Assembled on Tobacco Mosaic Virus Coat Protein

Ismael Abu-Baker, Amy Szuchmacher Blum, Anthony Mittermaier

McGill University

Abstract:

Bottom-up fabrication of precisely organized nanomaterials is a major challenge in materials science. Biological scaffolds show great promise as economical, monodisperse, programmable templates for synthesis of nanomaterials. Here we report the synthesis and characterization of highly organized arrays of gold nanoparticle (AuNP) rings assembled on a hexahistidine-tagged tobacco mosaic virus coat protein (6H-TMV-cp) template.

Near neutral pH, 6H-TMV-cp self-assembles into small disk-shaped particles. The His-tag is exposed on the outer edge of the disks and is available for interaction with other species in solution. Near pH 6.0, 6H-TMV-cp disks are known to self-assemble into 2D hexagonally-packed sheets of disks via His-His interactions. Here, we report two new nanostructures formed from 6H-TMV-cp disks: cubically-packed sheets, and nanotubes from rolled up hexagonally-packed sheets.

The His-tag also interacts strongly with gold nanoparticles to form rings of AuNPs around the disks. These AuNP rings are interesting because the plasmon bands of individual nanoparticles can couple together, leading to changes in the plasmonic effect within the radius of the ring.

Adding AuNPs to 6H-TMV-cp disks leads to the self-assembly of well-packed sheets of AuNP rings. When assembled on the nanotube structures, Au NPs form a hexagonal lattice around the surface, resembling a carbon nanotube. Characterization of the nanoring structures by transmission electron microscopy, small angle X-ray scattering, UV-vis spectroscopy, and dark field optical microscopy is underway to investigate both the physical structure and the plasmonic behaviour of the systems. Extended structures of well-organized plasmonic nanorings have many potential applications, including as sensors, metamaterial superlenses, and waveguides.

Thin-Film Polyimide Aerogels with Enhanced Mechanical Properties and Ultralow Dielectric Constant

Omid Aghababaei Tafreshi, Shahriar Ghaffari Mosanenzadeh, Zia Saadatnia, Chul B. Park, Hani E. Naguib

University of Toronto

Abstract:

Aerogels are a novel class of porous materials, which due to their highly porous nanostructured network exhibit ultrahigh thermal insulation properties as well as ultralow dielectric constant. Majority of research has been performed on inorganic aerogels (e.g., silica). However, as they lack mechanical flexibility, more recently, organic aerogels with improved flexibility have drawn a great attention. Organic aerogels are normally fabricated in bulk monolithic geometries and powder forms. However, the development of mechanically flexible thin-film aerogels with controlled dimensions and low dielectric constants has been a longstanding challenge. Thin-film aerogels have the potential to be used in the next generation of microelectronic devices, especially in electronics packaging. However, up to date, aerogels have not been employed in this field due to their inherent fragility and poor mechanical integrity. In this context, polyimide (PI) aerogels play an effective role. Compared to other inorganic and organic aerogels, PI is the only candidate satisfying all physical, chemical, thermal, mechanical, and electrical requirements of electronics packaging. In this study, we present a facile strategy for fabrication of thin-film PI aerogels, which not only exhibit enhanced mechanical properties, but also the dielectric constant remains ultralow. Combined with their excellent thermal stability, the developed products can be a promising alternative to currently available low dielectric constant materials in the microelectronics market. Demonstration of the application of these materials in microelectronics packaging is provided at the end.

Halloysite-reinforced polyurethane nanocomposite as an interlayer for transparent armour systems

Rafaela Aguiar, Ronald E. Miller and Oren E. Petel

Carleton University

Abstract:

In recent years, polyurethane (PU) formulations have been developed for new applications to increase the survivability of structures under high-strain-rate conditions, including against blast and ballistic loading events. PU coatings or interlayers are currently implemented in transparent armor systems as a way to increase the survivability of high-strength ceramic layers and improve fragment containment. Transparent armor must protect against blast and ballistic threats while maintaining structural integrity and optical transparency. Here, a PU nanocomposite interlayer is produced that significantly improves the ballistic resistance of multi-layered transparent laminates. The PU prepolymer is partially silane end-capped and filled with only 0.8 wt.% of acid-treated Halloysite nanotubes (HNTs). Ballistic testing results showed an increase on the ballistic limit, from 457 to 491 m/s, with the change from a neat PU interlayer to the nanocomposite. This large improvement, relative to the small concentration of HNTs cannot be attributed to the action of the HNTs as a simple reinforcing phase. Rater, our results elucidate the effect of the HNTs in the formation of the microstructural architecture of the PU. Molecular dynamics simulations were conducted to further investigate the effect of HNTs in the immiscibility and mobility of the segmented structure of the PU. Our simulation results suggest a greater degree of freedom of the soft segments in the nanocomposite, which can be understood as a consequence of the HNTs bonding to the hard segments, thereby encouraging the segregation of the hard segments from the mixed (hard and soft segment) matrix.

Metallurgical Grade Nano-Silicon Extracted and Process from Biomaterial Rice Husk

Benedict Ayomanor, Cookey Iyen, Daniel Dawuk, Ifeoma S. Iyen, Suleiman D. Ndiriza, Matthew Omonokhua, vitalis Mbah, Sunday A. Oricha

Federal Polytechnic Nasarawa, Federal University wukari

Abstract:

Rice husk (RH) a biomaterial waste product is found in large quantities in Nigeria and many other countries in Asia. This rich siliceous waste materials could yield valuable silica under controlled temperature and time. Its low production cost makes it most viable for preparing silica of high purity needed for metallurgical grade silicon. Nigeria alone would have the benefit of transforming its large volume (> 900,000 tonnes per annum) of biomaterial waste into a partial solution to the countrys issue with energy distribution. In this work, high purity silica (rice husk ash) ~ 99% has been prepared from RH ashed at 1000ºC for 5 hours by solid-liquid extraction (leaching) method. The rice husk ash (RHA) silica was leached with HNO3 and HCl solutions, followed by hydrometallurgical processes. The material was reduced via metallo-thermic process and characterized by X-ray fluorescence spectroscopy (XRF), X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy and Thermogravimetric (TG) analysis. The elemental analysis using XRF found major impurities are Fe2O3, K2O, Na2O, MgO, CaO, SO3, P2O5, Mn2O3, with Transmission Electron Microscopy analysis showing nanomaterial of 20nm.

Deformation mechanisms in concentrated solid solutions

Matthew Daly

University of Illinois at Chicago

Abstract:

Recent studies of multi-principal element and high entropy alloys have generated significant research interest in the metallurgy of concentrated solid solutions. From these efforts, it is now clear that the traditional theories of dilute alloys have several shortcomings in predicting the deformation behavior of systems with unusually large concentrations of alloying elements. In many cases, these shortcomings can be traced to the variations in solute interactions that arise from the unique topology of concentrated mixtures. In this talk, I will overview some recent progress in connecting the topological statistics of concentrated solid solutions with the emergent mesoscale plasticity mechanisms. This discussion will begin with a theoretical examination of the fluctuations in defect energies that emerge in concentrated mixtures, followed by a computational investigation of changes in deformation twinning mechanisms in systems with variable defect energies. Time permitting, some recent experimental work examining size effects in concentrated solid solutions will also be overviewed.

Determination of intrinsic fatigue toughness for predicting low-cycle fatigue behavior of aluminum alloys

Soumya Sobhan Dash, Dejiang Li (2), Xiaoqin Zeng (2), Dongyang Li (3), Daolun Chen (1)

(2) Shanghai Jiao Tong University, China; (3) University of Alberta, Canada; (1) Ryerson University, Canada.

Abstract:

Low iron-containing aluminum-silicon Silafont®-36 cast alloy exhibits improved ductility and superior strength. Automotive manufacturers have considered this alloy for the applications such as steering rods, engine cradles, shock tower components, etc. Understanding the low-cycle fatigue properties is essential for designing the load-bearing automotive structural components. As a result, the strain-controlled fatigue tests were conducted in this study, and the cyclic stress-strain hysteresis loops were analyzed in detail to evaluate the accumulated damage occurring in the material until failure under fully reversed cyclic loading at a strain ratio of R_ε=-1. Strain energy density or hysteresis loop area associated with each cycle was collectively taken into account to determine several fatigue parameters which were linked to the fatigue life of the alloy, like the intrinsic fatigue toughness, fatigue damage transition exponent, etc. A new method was developed to obtain these important parameters which were further used to improve fatigue life prediction models for the aluminum alloy. These parameters were also related to the heterogeneous microstructural features generated during the high-pressure die-casting, thus helping improve the understanding of cyclic deformation mechanisms. Details on this study will be presented at the conference.

Wear and mechanical behavior of hot-pressed alumina-based hybrid nanocomposites

Solomon Duntu

York University

Abstract:

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

Castability, Thermal/Electrical Conductivity, And Heat Treatability of Al-Fe-Ni Alloys

Abdallah Elsayed, Stephanie Kotiadis

University of Guelph

Abstract:

The changing requirements of automotive and aerospace manufacturers require alloys that are lightweight, electrically and thermally conductive, and castable. The addition of transition metals to Al alloys has demonstrated the potential to meet these requirements due to intermetallic strengthening. Castability is a general definition that encompasses properties such as hot tear susceptibility, die soldering, fluidity, and machinability. Heat treatability of alloys is also a concern as heat treatable alloys can demonstrate a range of properties including high conductivity, high strength, or high ductility. Alloys with the composition Al-(0.8-1.2) Fe-(0.2-0.6) Ni and varying amounts of Si and Mg have shown promising results with an electrical conductivity of more than 45 IACS% and hot tear susceptibility similar to that of typical Al-Si casting alloys. Permanent steel mold castings were used to quantifiably determine hot tear susceptibility and conductivity. Tensile samples were cast and heat treated to determine strength. The Weidman-Franz Law and an electrical conductivity meter were used to establish the electrical and thermal conductivity. The suspension of pure Fe wires in the Al-Fe-Ni melt were used to assess die soldering severity. By taking advantage of the low Al-Fe eutectic (1.8 wt.), Al alloys can achieve high castability through low hot tear susceptibility and die soldering. These alloys also demonstrate high electrical and thermal conductivity, moderate strength, and the ability to be heat treated. Overall, the Al-Fe-Ni system with Si and Mg additions provide the foundation for a new generation of casting alloys that considers the requirement for highly conductive transportation vehicle components.

Non-conventional Deep Cryogenic Treatment of Different Grades of Steel

Ehab Elsharkawi, Daniel Vincent, Jack Cahn, Mathieu Paré

Saint Mary's University, Deep Cryogenics International, Lunenburg, NS, Canada and Technosub, Rouyn-Noranda, QC, Canada

Abstract:

Deep cryogenic treatment (DCT) is a low-temperature treatment used to improve the mechanical properties of ferrous materials. This study investigating the effect of non-conventional protocol of deep cryogenic treatment on mechanical properties, electrical conductivity, and surface finish of non-heat-treated steel samples. The DCT process used in the current investigation consist of 8 hours ramp down from ambient to -190°C with slow cooling rate, 24 hours dwell at -190°C and 20 hours ramp up to ambient with slow heating rate using a low cost and highly effective setup. Five different grades of steel were used in the current investigation; cast iron and 304, 316, 420HC and 17-4ph stainless steels. All studied samples were deep cryogenically treated before testing. Hardness testing was carried out at room temperature using DigiRock DR3 Hardness Tester. Electrical conductivity and surface finish were carried out using Fischer Sigmascope SMP350 and Scanning White Light Interferometer, respectively. For all grades steel, results show that there is no significant change in the hardness and electrical conductivity between DCT treated and non-treated samples. However, DCT treated samples show an improvement of surface bearing area of 304SS and 17-4SS samples compared to non-treated condition. Tensile test was carried out at room temperature using MTS Servohydraulic mechanical testing machine. An improvement in the tensile properties of 304SS and cast-iron samples compared to the non-treated samples was observed.

Corrosion and nano/micro indentation hardness of electroplated Ni coatings from deep eutectic solvent containing SiO2 nanoparticles

Mehry Fattah, Sylvie Morin

York University

Abstract:

Wear and corrosion are two phenomena that happen during engineered component functionalities and result in deterioration of the component's surface. These phenomena lead to the failure of the surface protection characteristics and result in low in-service efficiency and increase in projected operation cost. In this work the effect of the addition of SiO2 nanoparticles into the Ni matrix with the goal of surface corrosion and hardness properties improvement is studied and discussed.

A choline chloride-ethylene glycol (ChCl:2EG)-based environmentally friendly deep eutectic solvent (DES), was employed to fabricate pure Ni and Ni-SiO2 nanocomposite coatings on the surface of AISI 1045 medium carbon steel through square waves pulse electrodeposition method at 70 °C and 8 mA.cm-2 current density of electrodeposition. Different amounts of 15 and 30 g/L of SiO2 nano powder were added to the electrolyte to produce Ni-SiO2 nanocomposite coating. SEM, XRD, XPS, nano/micro indentation hardness measurements, and potentiodynamic polarization test were used to study and characterize coatings microstructure, and corrosion and hardness properties. XRD results revealed Ni peaks at crystalline planes of (111), (200) and (220) for all coatings as expected. The presence of SiO2 in the coatings was detected by using EDX and XPS. High-resolution spectra for Ni 2p3/2 obtained from XPS on the surface of both pure Ni and Ni-SiO2 coatings consisted of metallic Ni, NiO, and Ni(OH)2 multiple peaks. Incorporation of SiO2 nanoparticles into the Ni matrix caused a decrease in Ni clusters size. Potentiodynamic polarization tests in 0.6 M aqueous NaCl solution at room temperature showed that the incorporation of SiO2 nanoparticles gave rise to the more positive corrosion potential and lower corrosion current density. Hardness was increased with the addition of SiO2 nanoparticles, and coating electrodeposited from the electrolyte containing 30 g/L SiO2 nanoparticles showed the maximum hardness.

An Investigation on the Influence of Composition Gradient on Interdiffusion Coefficient

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Abstract:

Solid-state diffusion has attracted significant attention for decades, due to its importance in materials processing and performance and the coefficient of interdiffusion is one of the key parameters required for quantifying it. Although the coefficient has been commonly considered as just a function of temperature and composition, the influence of composition gradient cannot be neglected, due to the possible effect of diffusion-induced stress (DIS). The present work is designed to experimentally investigate the influence of composition gradient on interdiffusion coefficient in the Ni-Cu system. To avoid the non-trivial errors that arise from the common assumption that the initial concentration profile is a step function in space, a new method that utilizes two composition profiles is used in the present work to calculate the interdiffusion coefficient. The results, which will be presented and discussed, confirm that; in contrast to what is commonly assumed, interdiffusion coefficient is not only a function of temperature and composition, but it can also significantly vary with composition gradient, due to DIS. This can have considerable effects on the theoretical prediction and analyses of diffusion process.

Thermal Stability of Nanocrystalline Electrodeposited Medium-Entropy Alloys

Michel Haché, Jason Tam, Uwe Erb, Yu Zou

University of Toronto

Abstract:

In the past decade, the field of complex concentrated alloys (CCAs) has drawn significant interest, particularly in the class of high-entropy alloys (HEAs, made up of 5 or more elements in roughly equal quantities). Such materials have exhibited peculiar mechanical, electrochemical, electrical, and magnetic properties owing, in part, to their complex, highly distorted structures. One particularly exciting finding from these studies is a heightened thermal stability, an issue that the nanocrystalline material community has struggled with for nearly half a century. This study examines the thermal stability of nanocrystalline medium-entropy alloys (MEAs, composed of 3 elements) made by electrodeposition, a fabrication process which lends itself well to scaling. Two exemplar systems were studied, NiFeCo and NiFeCr, each exhibiting improved thermal stability over nanocrystalline Ni and NiCo by ~100°C and ~75°C, respectively. Within these two systems, we also examine process-property-structure relationships as they relate to electrodeposition, revealing methods by which synthesis procedures can be tuned to maximize material performance. In this way, we have created a platform to take further advantage of CCA design, with aims of amplifying thermal stability through the development of 4- and 5-element electrodeposited nanocrystalline alloys.

Fe-containing Al Alloys for Applications in Electric Vehicles

Henry Hu

Dept. of Mechanical Engineering (MAME), University of Windsor

Abstract:

Iron is the main component of the earth's core, the most abundant element on the earth (about 35%), and it is relatively high in the sun and other stars. Also, it is a common and cheap metal in the manufacturing industry. Recently, with the rapid development of electric vehicles, more and more automotive companies are willing to develop new lightweight material for electric motors used in electrical vehicles. The iron–containing aluminum alloys can be considered as a good candidate, due to its great strength and electricity performance. This review describes various properties of aluminum-iron alloys including mechanical properties and electrical conductivities, as well their relation to the Fe contents. Also, metallurgical aspects of aluminum-iron alloys, including phase diagrams, equilibrium and non-equilibriun solidification, microstructure development, and castability. The further research and development work are outlined in terms of developing aluminum-iron alloys for some potential and value-added automotive applications.

The effect of annealing and impurities on the tensile properties of electroformed nanocrystalline Ni-Co alloy

Jonathan Kong, Jiahao Li, Jonathan L. McCrea, Jane Howe, Uwe Erb

University of Toronto, Integran Technologies Inc

Abstract:

The effect of annealing on the strength of an electroformed nanocrystalline Ni-32%Co alloy (grain size: 18nm) was examined by annealing the as-deposited material at various temperatures between 200℃-400℃ for one hour each. Increases in yield strength and ultimate tensile strength were observed in low temperature annealed samples (200 and 225℃) which can be attributed to grain boundary relaxation. The ductility of the as-plated and annealed samples at 200℃ are 6.6 and 5.7%, respectively. A significant drop in ductility for samples annealed at 225℃ to 3.8% coincided with the early stage of abnormal grain growth with ~3% abnormally grown grains (~100nm) in the structure. The reduction in ductility can be explained by accumulation of sulfur impurities along the grain boundaries of the abnormally grown grains that act as potential crack initiation and/or propagation sites within the material. The fracture surfaces revealed that ductile failure with dimple formation dominated in samples annealed at 250℃ and below. A mixture of dimples and cleavages was observed for samples annealed to 300℃ which reflects a transition from ductile to brittle fracture. This also corresponds to the late stage of abnormal grain growth with 90% abnormally grown grains. Significant segregation of sulfur impurities in samples annealed at 400℃ led to brittle intergranular fracture with faceted fracture surfaces. These results suggest that an improvement in the tensile properties of nanocrystalline Ni-32%Co can be attained by performing low temperature annealing on the material before abnormal grain growth takes place.

Microstructure and properties of graphene reinforced A356 aluminum alloy composites fabricated by gravity casting

Kyle Lessoway, Lava Kumar Pillari, Colin van der Kuur, Anthony Lombardi, Glenn Byczynski, Lukas Bichler

The University of British Columbia – Okanagan, ZenTek, NEMAK USA/Canada

Abstract:

The growing demand for more fuel-efficient vehicles continues to drive the development of aluminum (Al)-based components. Al alloy A356 has been often used in engine components, but the alloy is reaching its maximum operating temperatures due to the continued increase in engine temperature to enhance the efficiency of the combustion cycle. In the present study, graphene has been added as reinforcement into the A356 melt in the form of a master alloy. A356 composites with varying amounts of graphene have been fabricated by gravity casting. The obtained samples were characterized by optical microscope, scanning electron microscopy, Raman spectroscopy, and X-ray diffraction. In addition, various properties including hardness, tensile properties, the electrical and thermal conductivity of the composites was measured.

In situ monitoring of austenite grain growth and recrystallization with laser ultrasonics

Minghui Lin, Matthias Militzer

The University of British Columbia

Abstract:

The evolution of microstructure during complex thermomechanical treatments is of critical importance to the design of processing routes and the final properties of steel products. Compared to conventional time-consuming approaches such as metallography, laser ultrasonics enables rapid, real-time, and non-interrupted measurement of microstructure characteristics that can be related to the attenuation and velocity of the propagating ultrasound waves. Therefore, it provides a great opportunity for metallurgical studies involved in industrial rolling conditions including recrystallization, grain growth and phase transformation. The present work aims to utilize laser ultrasonics to quantify the microstructural changes involved in hot strip rolling for a Nb-microalloyed steel. The evolution of austenite grain size and static recrystallization after hot deformation is measured based on the correlation between grain size and the frequency dependence of ultrasound attenuation. The results from laser ultrasonics are compared with other techniques such as double-hit tests to demonstrate the capability of in situ monitoring under various conditions. Based on the experimental results, microstructural evolution models are proposed for hot rolling conditions..

Deformation and damage micromechanisms of Advanced High Strength Steels in bending

Nizia Mendes Fonseca, David Wilkinson, Jidong Kang

McMaster University, CanmetMATERIALS

Abstract:

The automotive industry has been challenged to improve passengers' safety and fuel efficiency concurrently. One way to address these two requirements is by developing so-called advanced high strength steels (AHSS), which enables a reduction in the component thickness without compromising the impact energy absorption of the automotive part. Despite having satisfactory strength and uniform elongation, AHSS show reduced formability, especially during tight-radius bending, with shear fracture being the dominant failure mechanism. Strain evolution during bending was evaluated at the macro and microscales. Three-point bending coupled with digital image correlation (DIC) was employed to assess the strain evolution at the macroscale. The strain distribution at the microscale was evaluated through quasi in-situ SEM bend testing coupled with DIC. The quasi in-situ testing technique enables the measurement of strain partitioning between the microstructural constituents and the identification of the micromechanisms leading to damage . During bending, the strain distribution is heterogeneous, with ferrite accommodating more deformation than other harder phases. The main damage micromechanism is decohesion of the interface between ferrite and martensite

Elucidating formation-structure-function relationships of Bioinspired Nanomaterials

Alana Ogata

University of Toronto

Abstract:

There remains a critical research gap regarding the rational design and controlled syntheses of bioinspired nanomaterials because their formation-structure-function relationships are unknown. This is largely due to the inherent challenges of studying nanomaterial formation and function. In nature, many biological materials form via complex formation pathways that include a diversity of nanoscale amorphous, crystalline, and protein phases and bioinspired nanomaterials exhibit similar formation mechanisms. Conventional bulk or dry-state analytical methods are insufficient for the identification of formation phases during material formation due to limitations in resolving heterogenous mixtures of species and analyzing hydrated phases in solution. In addition, limited control of bioinspired nanomaterial syntheses typically produces a distribution of particle sizes or structures that can result in heterogenous nanomaterial function and cannot be resolved by bulk analysis. Here, we study the formation and function of bioinspired nanomaterials using a new complementary approach that integrates cryotransmission electron microscopy (cryoTEM) and single-molecule fluorescence microscopy (SMF). Our preliminary work focuses on studying the structure-function relationships of metal-organic framework(MOF) nanozymes, which exhibit peroxidase activity. We show that changes in synthetic conditions result in a variety of MOF morphologies and catalytic activities. In addition, we investigated the role of heterogenous enzyme activity in enzyme-driven biomineralization of calcium phosphate. We show that alkaline phosphatase exhibits heterogenous activity using SMF and probe the relationship between enzyme activity and calcium phosphate structures.

Exploring microstructure evolution and thermal stability in response to high-temperature heat treatment of thin-strip cast AA5182 Al-Mg alloy

Hesam Pouraliakbar, L Andrew Howells, Mark Gallernaults, Vahid Fallah

Queen's University, Hazelett Castechnology Inc.

Abstract:

Thin-strip casting (TSC) process has been developed to fabricate thin gauge as-cast aluminum sheets (in the range of 2-5 mm) to be readily cold-rolled to final thicknesses which can efficiently address transportation industry demands. High fabrication speed and being cost-effective by eliminating intermediate thermomechanical steps of scalping, homogenization, hot-rolling, and annealing as well as being more environmentally friendly, make this novel method to be highly attractive and competitive with the conventional direct-chill (DC) casting. Due to the high production rate and thin thicknesses, high cooling rates could be achieved in as-cast products which generally result in a finer microstructure and supersaturated alloy matrix. Thus, rapid solidification could change the solute redistribution pattern and subsequently the formation kinetics of second-phase particles that in turn affect the alloy microstructure and mechanical properties, which are yet to be understood and optimized. In this study, the response of the supersaturated matrix in the TSC-AA5182 Al-Mg alloy to post-casting heat-treatment cycles in a wide temperature range of 150-600°C was investigated and compared with the results of conventional DC-AA5182 counterparts. The results revealed noticeably higher thermal stability of the TSC alloy in the experimented temperature range. Competing mechanisms of grain boundary migration and growth and precipitate formations were discussed and further confirmed through analytical modeling of the non-equilibrium solidification, microstructure characterization (via optical, scanning, and transmission electron microscopy techniques), and mechanical properties obtained by tensile and hardness measurements. According to the results, TSC-AA5182 alloy can be recommended for elevated temperature applications due to its microstructural stability that does not cause a noticeable loss in its mechanical characteristics.

In-Situ Investigation of Damage Mechanisms in a Duplex AlCoCrFeNi2.1 High Entropy Alloy

Cal Siemens, Dr. David Wilkinson

McMaster University

Abstract:

High entropy alloys (HEAs) have received much research attention due to their wide compositional range and variety of exceptional properties. The AlCoCrFeNi2.1 eutectic HEA (EHEA) is a microduplex casting alloy, consisting of face-centered cubic (FCC) and body-centered cubic (BCC) phases, which exhibits high strength and moderate ductility. Various studies have looked at the effects of thermomechanical processing routes on microstructure and basic tensile properties of this alloy. However, there is little work published on the fundamental mechanisms controlling damage and fracture, and no work investigating the change in these mechanisms after thermomechanical processing. An ingot of the AlCoCrFeNi2.1 HEA was cast using classical methods, and subsequently hot rolled. Scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS), and electron backscatter diffraction (EBSD) were used to characterize the resulting microstructures. Nanoindentation, SEM-based in-situ digital image correlation (μ-DIC) tensile testing, and x-ray computed tomography (XCT) were used to determine phase-specific mechanical properties and damage mechanisms. The as-cast EHEA fractured before work hardening was exhausted ($\varepsilon f = 0.16$), meanwhile the hot rolled EHEA ($\varepsilon f = 0.21$) exhausted work hardening and initiated ductile damage, but still showed limited post-uniform elongation. It was found that hot rolling significantly increased the ability of the EHEA to accommodate damage by delaying crack propagation and lowering phase strain partitioning at high strains, thus increasing phase co-deformation at high strain. We determined that micro-crack nucleation and propagation was a controlling fracture mechanism, and have identified the microstructural features that contribute to the increased ductility of the EHEA following rolling of the as-cast structure . Furthermore, this suggests methods to improve ductility in future HEA development.

Statistical distribution of spontaneous recombination radii of Frenkel pairs in FCC and BCC metals

Hao Sun, Laurent Karim Béland

Queen's University

Abstract:

The recombination radius of Frenkel pairs generated by incident high-energy particles represents a critical determinant of irradiation-induced microstructure evolution. Mesoscale models of radiation damage evolution that include recombination radii as input parameters can benefit from a better understanding of the atomistic processes controlling recombination. This work used the kinetic activation relaxation technique—an off-lattice, self-learning kinetic Monte Carlo algorithm—in conjunction with molecular dynamics simulations, to study the statistical distribution of the recombination radii in four FCC (nickel, copper, silver, and platinum) and one BCC (iron) structures. We found that recombination can occur from the 2nd nearest neighbor site (neighbor site) to as far as the 18th neighbor site. Such long-range recombination is realized via the formation of crowdions. Vacancies were found to have no effect on interstitial migration, aside from diminishing the recombination energy barriers, which are linearly related with diffusion energy barriers. No correlation was found between energy barriers and recombination radii. Instead, because the interatomic interaction in high-stacking-fault-energy metals has a directional character akin to covalent bonds, the deformation near self-interstitials distributes mainly along the closest packed directions. As a result, crowdions more readily form between Frenkel pairs at longer distances, resulting in larger recombination radii. Similarly, hydrostatic pressure enhances the recombination radius by extending the distortion induced by self-interstitials along the closest packed directions. Thus, the deformation distribution near self-interstitials is the determining factor controlling recombination radii, not energy barriers.

Investigating Structure-function relationships in Copper Bypyridine Metal-Organic Framework for Rational Design of Nanozymes

Justin Van Houten, Alana Ogata

University Of Toronto Mississauga

Abstract:

Metal organic frameworks (MOFs) are an important type of material that have promising applications in catalysis, energy technologies, and analytical chemistry. One of the unique properties of MOFs is the use of these materials for mimicking enzymatic activity, often referred to as “nanozymes”. One such nanozyme is copper bipyridine (Cu-Bpy) MOFs. CuBpy MOFs are known to mimic the activity of peroxidase enzymes, such as horseradish peroxidase. However, the structural properties that give rise to the mimetic activity of Cu-Bpy is not well understood. To address this challenge, an investigation was done to provide new insights into the structure-function relationship of catalytically active MOFs. Cu-Bpy MOFs were synthesized using various precursor concentrations, Cu: Bpy precursor ratios, temperatures, and solvent conditions. Under aqueous synthetic conditions, Cu-Bpy MOFs were observed to undergo significant structural alterations. Here, increasing absolute precursor concentration resulted in significantly smaller particles, when compared to a standard (4:16, Cu:Bpy), as observed by a transition from µm to nm sized particles. Phase transition from baculite-type mircostructures to new morphological configurations such as microsheets, nanomills, nanopills, and microfilbrils, were observed using high reaction temperatures and different solvent conditions. The peroxidase activity of the resulting Cu-Bpy MOFs was subsequently evaluated using TMBox assay. Differing Michaelis-Menten kinetics were observed within the group of Cu-Bpy MOFs. These new catalytic parameters suggests that differences in structure can alter properties of nanozyme MOFs, analogous to their enzymatic counterparts.

Development and characterization of multi-principal element alloys with superior mechanical properties and irradiation resistance

Haiming Wen, Matthew Luebbe, Hans Pommerenke

Missouri University of Science and Technology

Abstract:

Conventional alloy design based on single-principal element systems limits the space and flexibility to explore alloy chemistries and optimize microstructures. The concept of multi-principal element alloys (MPEAs, or high-entropy alloys) has revolutionized traditional alloy design strategies, creating tremendous opportunities to explore new alloys in the vast compositional space. Some MPEAs have been reported to possess significantly improved mechanical properties over conventional alloys, such as high strength-weight ratio, fracture resistance, high-temperature strength and structural stability. However, the specific properties depend on the specific composition, processing and microstructure, and the composition-process-structure-property relationships need to be well understood. Furthermore, MPEAs have been proposed to possess significantly enhanced irradiation tolerance. Nevertheless, irradiation studies of MPEAs (especially precipitation-strengthened ones) are limited and mechanisms underlying irradiation behavior remain poorly understood. Most MPEAs developed so far contain Co, which are not suitable for nuclear applications. In this study, solid-solution or precipitation-strengthened MPEAs with different compositions (including Co-free ones) and microstructures were processed by conventional manufacturing (casting followed by rolling and heat treatment) or advanced manufacturing techniques (including powder metallurgy route involving rapid sintering, and severe plastic deformation). The microstructure of the fabricated MPEAs were carefully studied utilizing advanced microstructural characterization techniques. Mechanical properties and irradiation behavior were investigated. Results indicated that excellent mechanical properties including high-temperature strength were achieved, as well as enhanced irradiation tolerance. This study provides insights to optimize the design and processing of MPEAs to achieve superior mechanical and physical properties.

Mechanical characterization and additive manufacturing of metals across scales

Yu Zou

University of Toronto

Abstract:

Throughout history, exploration of material properties at different length scales, both large and small, have fundamentally reshaped human understanding of the physical world and catalyzed industrial growth. Towards this vision, my seminar will focus on mechanical properties of materials in the size ranging from a few micrometers to about one hundred nanometers. I will first explain a well observed phenomenon – "smaller-is-stronger". Then, I will share insights on mechanical characterization of emerging nanostructured refractory high-entropy alloys: I achieve mechanically strong (yield strength of ~10 GPa) and thermally stable (after annealing at 1100 °C for 3 days) nanocrystalline alloys, surpassing conventional nickel-based superalloys and pure tungsten. In addition to small-scale mechanics, I will talk about my research on metal additive manufacturing (3D printing) techniques – selective laser melting in which fast melting and solidification of metal powder result in bulk components, as well as cold spray and RF Plasma spray. In closing, I will talk about future research directions of my group about the combinatorial development of structural materials.

Development of a Novel Cobalt High-Entropy Alloy for Wear/Corrosion Resistance

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Abstract:

In this research, a novel high-entropy alloy (HEA) having the equiatomic Co-Cr-Fe-Ni composition with high W (>18 wt pct), low C (<1 wt pct) and minor Mo contents, is created by combining the features of HEA and Stellite alloy, which is designated as HE6. The bulk specimens of HE6 are fabricated from the alloy powder via spark plasma sintering (SPS) or plasma transferred arc (PTA) welding process. The microstructural analyses using SEM/EDX/XRD reveal that HE6 has a microstructure consisting of diverse carbides and intermetallics embedded in a solid solution matrix which is constituted with multiple element FCC structures. The hardness and dry-sliding wear tests show that HE6 does not perform as well as Stellite 6 which is the benchmark of Stellite alloys. Under the electrochemical and immersion corrosion tests in hydrochloric acid and sulfuric acid, HE6 displays passivation ability by forming protective Cr oxide films, but localized corrosion (pitting) can occur when the oxide films are broken. HE6 exhibits lower corrosion rates under the immersion test in hydrochloric acid and sulfuric acid for the longer testing duration (72 hours), compared to Stellite 6, also shows nearly stable corrosion rate with testing duration extended, indicating better repairing ability of the oxide films.

How nanograins form at high strains and strain rates

Ahmed A. Tiamiyu

Department of Mechanical and Manufacturing Engineering, University of Calgary, 2500 University Drive NW, Calgary, Alberta T2N 1N4, Canada.

Abstract:

During the deformation of FCC metals, grain refinement by dynamic recrystallization is usually explained by classical dislocation-mediated mechanisms—discontinuous and continuous dynamic recrystallization. However, these classical mechanisms do not explain grain evolution at the nanoscale, especially in extreme processes that involve high strain and strain rate (low temperature) where twinning is the dominant plastic deformation mechanism. This talk explains how single copper microparticle impact experiments at varying velocities are employed to systematically access these extreme regimes. Post-mortem characterization of impact sites reveals a new mechanism of grain refinement—nanotwinning-assisted dynamic recrystallization (ntDRX). In the ntDRX mechanism, nanotwins first form and are then partitioned by dislocation activity to form nano-grains smaller than what conventional dislocation-mediated recrystallization mechanisms produce. This finding fills in the gaps at high strains and strain rates in a deformation mechanism map for FCC copper.

Posters:

Fatigue behavior of an Al-Si alloy under symmetric and asymmetric cyclic deformation.

Soumya Sobhan Dash, Dejiang Li (2), Xiaoqin Zeng (2), Dongyang Li (3), Daolun Chen (1)

(2) Shanghai Jiao Tong University, China; (3) University of Alberta, Canada; (1) Ryerson University, Canada.

Abstract:

Strain-controlled low-cycle fatigue tests can be carried out at varying sequences and strain amplitudes by changing strain ratio (Rε) values ranging from negative infinity to nearly positive one (+1). This can further be classified as symmetric and asymmetric cyclic loading conditions. Fatigue life of a high-pressure die-cast Al-Si alloy was determined under strain control at a constant total strain amplitude of 0.4% and varying strain ratio values from negative infinity to +0.5 in this study and the relevant influencing factors associated with the changes were analyzed. This low iron containing Silafont®-36 cast alloy constituted a fibrous-coral like network of strontium modified-Si particles, which were embedded in the Al matrix somewhat like a particulate-reinforced composite. It also contained some magnesium and manganese alloying elements, being necessary to improve the strength and fatigue properties and replace part of iron which could lead to brittle intermetallic phases. Mean stress in this alloy showed a significant relaxation at different strain ratio values and was responsible for the change in the fatigue life. A power law based new equation was proposed to describe nicely the trajectory of the mean stress relaxation. Cyclic hardening degree was also evaluated at different strain ratios, which showed a significant change. Further details will be presented at the conference.

Castability, Thermal/Electrical Conductivity, And Heat Treatability of Al-Fe-Ni Alloys

Abdallah Elsayed, Stepahnie Kotiadis

University of Guelph

Abstract:

The changing requirements of automotive and aerospace manufacturers require alloys that are lightweight, electrically and thermally conductive, and castable. The addition of transition metals to Al alloys has demonstrated the potential to meet these requirements due to intermetallic strengthening. Castability is a general definition that encompasses properties such as hot tear susceptibility, die soldering, fluidity, and machinability. Heat treatability of alloys is also a concern as heat treatable alloys can demonstrate a range of properties including high conductivity, high strength, or high ductility. Alloys with the composition Al-(0.8-1.2) Fe-(0.2-0.6) Ni and varying amounts of Si and Mg have shown promising results with an electrical conductivity of more than 45 IACS% and hot tear susceptibility similar to that of typical Al-Si casting alloys. Permanent steel mold castings were used to quantifiably determine hot tear susceptibility and conductivity. Tensile samples were cast and heat treated to determine strength. The Weidman-Franz Law and an electrical conductivity meter were used to establish the electrical and thermal conductivity. The suspension of pure Fe wires in the Al-Fe-Ni melt were used to assess die soldering severity. By taking advantage of the low Al-Fe eutectic (1.8 wt.), Al alloys can achieve high castability through low hot tear susceptibility and die soldering. These alloys also demonstrate high electrical and thermal conductivity, moderate strength, and the ability to be heat treated. Overall, the Al-Fe-Ni system with Si and Mg additions provide the foundation for a new generation of casting alloys that considers the requirement for highly conductive transportation vehicle components.

High Manganese Press Hardenable Steel for Automotive Safety Applications

Sara Kheiri, Dr. Joseph McDermid

McMaster University

Abstract:

Press-hardened steels (PHS) are widely used in the Body-In-White of cars as they promote passenger safety and, due to their lower weight, reduce vehicle emissions. Al-Si coated 22MnB5 family of alloys are mainly utilized in the direct hot press forming (DHPF) process. Zn coatings, however, are promising as they can have superior corrosion protection and a lower cost. Liquid Metal Embrittlement (LME) is one of the challenges faced by the implementation of zinc-coated DHPF steels, which is caused by stamping above the Fe-Zn peritectic temperature of 780 °C during press forming. A PHS grade with 2% Mn content has been suggested that avoids LME by allowing stamping at lower temperatures. The objective of this study was to determine the feasibility of DHPF processing a galvannealed coating on a substrate with the composition of 0.19C-1.92Mn-0.2Si-0.03Ti-0.003B (wt%) in line trials of the automotive industry. Therefore, a process window comprising of annealing for 120 s at 890 °C and stamping temperature of 550 °C to 700 °C for this substrate was determined that effectively avoids LME. Moreover, this process windows meets the ultimate tensile strength (UTS) objective of >= 1500 MPa.

Hydrogen Embrittlement of Iron

Aynour Khosravi, Normand Mousseau & Jun Song

Universite de Montreal, McGill University

Abstract:

Hydrogen embrittlement(HE), the process by which a material is caused to fail prematurely

when exposed to hydrogen, has haunted the metal design and application industry since its

discovery over a century ago while the exact mechanisms underlying the occurrence of HE

remain a mystery despite an extensive research effort on the HE.

Despite the wealth of existing research, rational design criteria and accurate long-term assessments of steels against HE remains scarce, this is because the mechanistic details on H diffusion and segregation within microstructures remain unclear.

Previous studies on HE have mostly focused on equilibrium or close to equilibrium situations, with little attention being paid to the important role played by kinetics. Consequently, new strategies are required to predict the various H trap states and key mechanisms of H kinetics.

Here, we use the kinetic Activation-Relaxation Technique (k-ART), an off-lattice kinetic Monte Carlo approach with on-the-fly event catalog building, to help us address the challenging problem in this subject. Simulations using k-ART are able to provide migration barriers, long-term diffusion paths, and collective diffusivities of H on microstructures without bias, including elastic effects both at short and long ranges, as well as complex environments.

We investigate how hydrogen atoms diffuse in perfect BCC iron as well as in structures with defects as vacancies and grain boundaries, using k-ART simulations, so we can determine diffusivities and diffusion barriers for hydrogen atoms moving. Normally,

hydrogen diffuses too fast with a small energy barrier, but in presence of vacancy, it is strongly trapped. Further evidence shows that hydrogen atoms bind strongly to defects, rather than other hydrogen atoms. Results show that the mechanisms for diffusion of hydrogen are altered at vacancies, dislocations, and grain boundaries and shed light on the understanding of the behaviour of H in iron and the HE mechanism.

Effect of graphene on the microstructure and properties of as-cast B319 aluminum alloy

Lava Kumar Pillari, Kyle Lessoway, Colin van der Kuur, Anthony Lombardi, Glenn Byczynski, Lukas Bichler

The University of British Columbia-Okanagan, Kelowna, Canada, Zentek Ltd., Thunder Bay, Canada; Nemak USA/Canada, Windsor, Canada

Abstract:

Global trends in the automotive and aviation industries target lighter vehicles driven by stringent fuel standards aiming to reduce greenhouse gas emissions. The B319 aluminum alloy is most commonly used in automotive powertrain applications due to its low density, good strength, and excellent castability. However, the strength of B319 alloy degrades at the engine's operating temperature caused by precipitate coarsening and insufficient thermal conductivity. In this research, B319 alloy composites reinforced with various graphene amounts were developed through the combination of solid-state (powder metallurgy) and liquid-state (casting) routes. The effect of graphene addition on the microstructure of as-cast B319 alloy was studied by Raman spectroscopy, X-ray diffraction, optical microscopy, and scanning electron microscopy. Furthermore, the mechanical properties (hardness and tensile strength), thermal and electrical conductivity of the composites were evaluated.

In-situ studies of inclusions separation at the molten steel- slag interface

Guang Wang, Muhammad Nabeel, Neslihan Dogan

McMaster University

Abstract:

Studying the separation of inclusions at the molten steel-slag interface is of critical important for a better control on both the size and the number of inclusions, as well as improving the stability of continuous casting process and the quality of steel products. In this study, the behavior of inclusions at the interface of molten steel-slag was observed in-situ with using High Temperature Confocal Laser Scanning Microscopy (HT-CLSM) equipped with a gold-image furnace. At the molten steel-slag interface, solid irregular, semi liquid and liquid spherical inclusions were observed, and they were found to react with slag . Different behaviors of different shape and size inclusions were observed. Those different behaviors caused by the composition, size and contact angle.

Exploring microstructure evolution and thermal stability in response to high-temperature heat treatment of thin-strip cast AA5182 Al-Mg alloy

Hesam Pouraliakbar, Andrew Howells, Mark Gallernaults, Vahid Fallah

Queen's University, Hazelett Castechnology Inc.

Abstract:

Thin-strip casting (TSC) process has been developed to fabricate thin gauge as-cast aluminum sheets (in the range of 2-5 mm) to be readily cold-rolled to final thicknesses which can efficiently address transportation industry demands. High fabrication speed and being cost-effective by eliminating intermediate thermomechanical steps of scalping, homogenization, hot-rolling, and annealing as well as being more environmentally friendly, make this novel method to be highly attractive and competitive with the conventional direct-chill (DC) casting. Due to the high production rate and thin thicknesses, high cooling rates could be achieved in as-cast products which generally result in a finer microstructure and supersaturated alloy matrix. Thus, rapid solidification could change the solute redistribution pattern and subsequently the formation kinetics of second-phase particles that in turn affect the alloy microstructure and mechanical properties, which are yet to be understood and optimized. In this study, the response of the supersaturated matrix in the TSC-AA5182 Al-Mg alloy to post-casting heat-treatment cycles in a wide temperature range of 150-600°C was investigated and compared with the results of conventional DC-AA5182 counterparts. The results revealed noticeably higher thermal stability of the TSC alloy in the experimented temperature range. Competing mechanisms of grain boundary migration and growth and precipitate formations were discussed and further confirmed through analytical modeling of the non-equilibrium solidification, microstructure characterization (via optical, scanning, and transmission electron microscopy techniques), and mechanical properties obtained by tensile and hardness measurements. According to the results, TSC-AA5182 alloy can be recommended for elevated temperature applications due to its microstructural stability that does not cause a noticeable loss in its mechanical characteristics.

Defects and Quantum States based on Bi/Si(111) System

Longxing Chi, Chandra Veer Singh, Jun Nogami

University Of Toronto

Abstract:

Bi/Si(111)-$\sqrt{3}\times\sqrt{3}$ surface reconstruction is a promising 2D system for spintronic fabrication and spin current control due to its extraordinary Rashba spin splitting.[1] Previous report has already covered the crystal and electronic structures of the system.[2] However, potential applications in quantum devices using its unique electronic states have rarely been mentioned. Here, we investigate the influence of defects and potential quantum applications of Bi/Si(111)-based 2D systems using scanning tunneling microscopy and density functional theory. First, connection between in-gap surface states and defects in the Bi/Si(111) system is interpreted. Analysis on the defect states perfectly convince the origin of in-gap surface states. Second, phase transition induced quantum dot states are observed on the Bi/Si(111) system, which can be easily achieved by thermal annealing. The quantum dot size can also be predicted by a kinetic fitting model during the transition. Finally, a $2\sqrt{3}\times2\sqrt{3}$ Pb superlattice can be achieved on the Bi/Si(111) surface, which exhibits strong Rashba splitting and can be used to fabricate quantum well devices.

[1] Liang, Q.-F.; Yu, R.; Zhou, J.; Hu, X., Topological states of non-Dirac electrons on a triangular lattice. Phys. Rev. B 2016, 93 (3). [2] Hsieh, S.-C.; Hsu, C.-H.; Chen, H.-D.; Lin, D.-S.; Chuang, F.-C.; Hsu, P.-J., Extended α-phase Bi atomic layer on Si(1 1 1) fabricated by thermal desorption. Appl. Surf. Sci. 2020, 504.

Mitigating vdW Dominated Fatigue Damage of 2D Materials on Flexible Substrate

Md Akibul Islam, Boran Kumral, Guorui Wang, Teng Cui, Peng Pan, Xinyu Liu, Tobin Filleter

University of Toronto

Abstract:

Graphene and other 2D materials are often in contact with stretchable polymer substrates in applications like flexible electronic devices. Such devices are often subjected to dynamic mechanical loading which can eventually deteriorate the weak vdW interface between the 2D material and the polymer substrate. This can lead to significant local delamination and shear fracture of the 2D materials, in particular when the graphene is not capped with polymer. Using a polymer encapsulation method, we have shown that the damage in multilayer graphene (MLG) is significantly mitigated when capped. We have used in situ optical microscopy cyclic loading to observe the damage propagation in non-encapsulated and encapsulated MLG. The standard shear lag model is used to explain the underlying mechanism behind this significant improvement. We further found that softer polymer substrates are more effective in mitigating local delamination due to their stronger adhesion with MLG compared to stiffer polymers.

Role of Prefactors in Point Defect Diffusion in 55Fe-28Ni-17Cr Solid Solution Alloy: A Dynamical Study with the kinetic Activation-Relaxation Technique (k-ART)

Joseph Lefèvre, Gilles Adjanor, Christophe Domain, Normand Mousseau

Université de Montreal, EDF Lab Les Renardières

Abstract:

High entropy alloys and concentrated solid-solution alloys (CSAs) have attracted considerable attention over the last years for their unexpected properties. Among those is a slower defect diffusion rate with respect to pure elements and conventional alloys, a property that would lead to higher resistance to neutron radiation. Here, we use the kinetic Activation-Relaxation Technique (kART), an off-lattice kinetic Monte-Carlo algorithm with on-the-fly catalogue building, to explore the origin of this slower diffusion. We focus here on the 55Fe-23Ni-17Cr CSA, described by Bonny's FeNiCr-2013 EAM potential.

The transition rate of events is obtained using the Arrhenius equation, in which the pre-exponential factor is often approximated to be constant. However, in this study the prefactors were computed using the harmonic transition state theory (HTST), a method that uses the ratio between vibrational frequencies at the initial minimum and at the saddle point. This will allow to analyze the impact of prefactors on the dynamics of defect diffusion in CSAs.

While the observed energy barriers are the same regardless of how prefactors are evaluated, the HTST prefactor distribution covers several orders of magnitude. Their value varies a lot between events, even when the barriers have similar amplitudes. Then, when observing their value on selected events only, the distribution keeps roughly the same width, with an average slightly under 10E13 Hz. This allows the system to visit more events with high energy barriers than in constant prefactor simulations.

This difference has an impact on the kinematics of the system. We observe that while the constant prefactor simulations tend to heavily prioritize Cr atom displacements, the transition state method allows to access more events centered on a Fe or Ni atom, affecting the overall diffusion of the system.

Sustainability and CO_2 capture

Oral Presentations:

Individual metal separation during recycling of end-of-life lithium-ion batteries using electrodialysis

Ka Ho Chan, Monu Malik, Gisele Azimi

University of Toronto

Abstract:

This study aims to separate and recover lithium, nickel, manganese, and cobalt from LiNi0.33Mn0.33Co0.33O2 chemistry of lithium-ion batteries using a three-stage electrodialysis. Before the electrodialysis experiment, the complexation of ethylenediaminetetraacetic acid (EDTA) with four different metals is investigated using ultraviolet-visible spectroscopy. During the three-stage electrodialysis experiment, nickel is separated in stage 1 and cobalt is then separated in stage 2 using electrodialysis coupled with EDTA. Subsequently, lithium is separated from manganese in stage 3 using electrodialysis with a monovalent cation-exchange membrane. After the electrodialysis experiment, nickel and cobalt are decomplexed from EDTA at pH below 0.5 and all four metals are recovered using selective precipitation. This study demonstrates that using the three-stage electrodialysis process to separate four different metals in the multi-metallic system is feasible and could be potentially utilized in other industries that involve the waste valorization of critical metals.

Breaking the scaling relation: rotation on high entropy alloy catalysts for CO2 reduction reaction

Zhi Wen Chen, Chandra Veer Singh

University of Toronto

Abstract:

The rapid increase in global energy demand and the need to replace carbon dioxide (CO2)-emitting fossil fuels with renewable sources have driven interest in chemical storage of intermittent solar and wind energy. Particularly attractive is the electrochemical reduction of CO2 to chemical feedstocks through utilizing both CO2 and renewable energy. However, the catalytic efficiency of CO2 reduction reaction (CO2RR) is limited by the scaling relation between adsorption intermediates during the reaction process. Breaking the scaling relation is the only available strategy to achieve a breakthrough in catalytic performance of CO2RR. In this work, based on density functional theory (DFT) calculation, we designed a high entropy alloy (HEA) system of FeCoNiCuMo with high catalytic activity for CO2RR. Machine learning models were developed by ~1000 datapoints achieved by DFT calculations to predict the adsorption energy of COOH*, CO* , and CHO*. The scaling relation between the adsorption energies of COOH*, CO*, and CHO* is broken on the designed HEA surface, resulting into the outstanding catalytic activity of CO2RR. This work not only accelerates the development of HEA catalysts, but also provide a new strategy to break the scaling relation.

Supercritical Carbonation of Electric Arc Furnace Slag: Process Development and Mechanistic Investigation

Jihye Kim, Gisele Azimi

University of Toronto

Abstract:

Mineral carbonation of steelmaking slag has proven to be a compelling carbon capture and storage technique to mitigate anthropogenic carbon dioxide (CO2) emissions while stabilizing steelmaking slag and producing enhanced construction materials. Significant amounts of CO2 emitted from the steelmaking process can be sequestered at the point sources using the slag carbonation, reducing the overall CO2 gas emissions and offering the environmental benefits of waste reduction. The current study is focused on developing an efficient and environmentally sustainable supercritical carbonation process to sequester CO2 using the byproduct of the steelmaking industry. A response surface methodology is utilized to develop an empirical model for calculating the carbonation efficiency as a function of operating parameters, which in turn, enables process optimization. With systematic experimental approaches and fundamental investigations, the carbonation mechanisms are elucidated with the emphasis on the type and thickness of diffusion barrier, rate-determining step, and reaction pathway. The developed process offers the advantage of high carbonation efficiency (213 gCO2/kgslag), fast kinetics, no use of chemicals, and minimal volumes of waste. We believe the findings of this study would help enable efficient CO2 mitigation utilizing an efficient and environmentally sustainable process and thereby contribute to carbon neutrality, sustainable systems engineering, and waste valorization.

Study of Spinel-Structured $ZnFe_2O_4$ as a Low-Temperature CO_2 Splitting Agent

Mengsha Li, Yangfan Xu, Chenyue Qiu, Stas Dogel, Hooman Hosseinkhannazer, Doug Perovic, Geoffrey A. Ozin, and Jane Howe

University of Toronto

Abstract:

Carbon dioxide (CO_2) is a greenhouse gas and its continuous increase in the atmosphere results in the global warming issue. An appealing solution to alleviate CO_2 emissions is to convert them into value-added products such as fuels and daily chemicals products, such as solar-driven thermochemical CO_2 reduction. However, this process requires a very high operation temperature. Herein, we demonstrate a low-temperature CO_2 splitting method by using zinc ferrite ($ZnFe_2O_4$) with hydrogen.

In this work, we performed the in situ gas scanning transmission electron microscopy (STEM) to study $ZnFe_2O_4$ nanoparticles in the CO_2 reduction process. The experiment was conducted using Norcada's micro-electromechanical systems (MEMS)-based chips in Hitachi Blaze heating-gas holder inside an environmental transmission electron microscope (ETEM, Hitachi HF-3300). The CO_2 reduction process was achieved by exposing to hydrogen and CO_2 gases, and all the reactions were at 300 °C. During the redox reaction, the lattice extracted from the particle centre region remains at about 2.55Å. Interestingly, when the nanoparticles are exposed to H_2, the lattice expands to 2.70Å at the surface region and then shrinks to the original value in the CO_2 atmosphere.

In addition to the structural changes, the dynamic observation of chemical reactions could be also achieved by combining STEM imaging with electron energy-loss spectroscopy (EELS). The intensity ratio (L3/L2) of the Fe L3 and L2 white lines are used to measure the oxidation number of Fe. After calculation, L3/L2 decreases to 4.04 in H_2 and then increases to 4.64 in CO_2. This result indicates that H_2 can partially reduce the Fe(III) to Fe (II) on the sample surface, while the original oxidation state of Fe can be recovered when exposing to the CO_2 environment as a result of a CO_2 reduction reaction. Our findings suggest that $ZnFe_2O_4$ can be used as a cost-effective material for low temperature CO_2 conversion.

Extraction of Rare Earth Elements from an Ore Concentrate Using Supercritical Carbon Dioxide

Sicheng Li, Monu Malik, Gisele Azimi (Corresponding)

University of Toronto

Abstract:

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In recent years, a steady, reliable, and secure supply of critical metals has become increasingly important to major industrialized economies such as clean energy. Rare earth elements (REEs) represent an opportunity to enter an emerging and globally strategic market. The current REE extraction processes, i.e., pyrometallurgy and/or hydrometallurgy, face environmental challenges such as air pollution emissions and large amounts of hazardous waste production. Thus, it is highly desirable to develop an environmentally sustainable extraction process. In this study, an emerging green process called supercritical fluid extraction (SCFE) is developed to extract REEs from an ore concentrate. Supercritical CO2 and a small volume of a chelating agent (tributyl phosphate-nitric acid) are as the solvent. The CO2 solvent can be easily separated from the products through depressurization and recycled back to the process. In addition, a pretreatment method based on sodium hydroxide (NaOH) cracking is introduced to enhance the SCFE efficiency. A systematic study under a wide range of operating conditions is conducted and the process optimization for both processes (NaOH cracking and SCFE) is carried out, which results in more than 90% extraction efficiency. The process mechanism is also elucidated through fundamental studies and advanced characterizations. The results of this study enable the development of an efficient and environmentally sustainable REE extraction process.

Production of high purity lithium hydroxide using barium hydroxide

Hongting Liu, Gisele Azimi

University of Toronto

Abstract:

Lithium hydroxide monohydrate (LiOH ⋅H2O) is a critical precursor for the production of the current most popular NMC (nickel-manganese-cobalt) type lithium ion batteries. The lithium industry face the challenge of producing high purity LiOH ⋅H2O with high yield. In this study, a method for the production of battery grade lithium hydroxide monohydrate from lithium sulfate (Li2SO4) solution (leached from ores) by using barium hydroxide (Ba(OH)2) is proposed. Various operating parameters are investigated and under the best conditions, more than 90% of lithium in the concentrated Li2SO4 system is converted to the LiOH ⋅H2O with over 99.5% purity in a one-step sonication-assisted process. Additional washing and carbonation steps are also introduced to further improve the product yield and purity. The byproduct barium sulfate (BaSO4) is recycled and used to reproduce the Ba(OH)2 reagent, which reduces the environmental impact and enhances the economic efficiency. It is expected this study would help the lithium industry improve the production of high quality LiOH ⋅H2O from lithium resources in a sustainable and efficient manner.

Tailoring KOH Activated Carbon Materials by Transforming Micropores via Heat Cycling and its effects on naphthenic acids adsorption

Oliver Strong, Andrew Vreugdenhil, Tyler Roy, Elmira Nazari

Trent University

Abstract:

Formation of activated carbon from petroleum coke by KOH, results in high surface area materials that are predominantly microporous. This microporosity limits the field of application that such a product can be used in, as the resulting adsorption kinetics are slow. To address this problem a series of additional heat cycles with no additional chemical inputs were applied after activation but prior to removal of activating agents. This heat cycling resulted in an increase in mesoporosity by 10-25 % with each successive cycle independent of the KOH to feedstock ratio. This was shown to be demonstrably different than equivalently extended heating times continuously thus identifying the importance of thermal cycling. Adsorption kinetics of three model naphthenic acids were examined for the pore widened activated carbon showing faster kinetics as pore width increased.

Nickel extraction from sulfide nickel ores with minimal sulfur dioxide emissions

Fanmao Wang, Sam Marcuson; Mansoor Barati

University of Toronto

Abstract:

Ni is a strategic metal in modern society. The primary use of Ni is in stainless steel. Recently, the use of Ni in lithium ion battery is increasing. Laterites and sulfides are the major ores for Ni production. Ni extraction from sulfides begins with smelting of the concentrates to remove Fe and S as iron oxide and sulfur dioxide. The abatement of SO2 emissions is in instances even more expensive than smelting , resulting in the shutdown of smelters. The smelting product is matte, not marketable and requires complex refining to produce metallic Ni.

The authors proposed a simple extraction method with minimal SO2 emissions and less refining treatment. Heating metallic Fe and Ni sulfide concentrates at elevated temperatures under Ar, Ni is extracted into ferronickel (FeNi) alloy while leaving S as solid iron sulfide. Further, a two-stage thermal treatment was proposed to obtain high Ni extraction and large FeNi grain size simultaneously. The first stage temperature is low enough to avoid entire melting but high enough to create a certain amount of liquid that facilitates large FeNi size. The second stage is at lower temperatures for high Ni extraction. When Fe addition to Ni sulfide concentrate was 0.5 and temperatures were 950-800 ⁞C, 95% Ni extraction was obtained with 39% Ni grade and a grain size of d80=106 µm. After magnetic separation, Ni recovery was 93%, Ni grade was 30%, and the remaining S was 4%. This product can be desulfurized and supplied to stainless steel. Alternatively, it can be converted into suitable intermediate to produce Ni-cathode.

The proposed method avoids smelting, hence appears promising to process ultramafic Ni sulfides. The ultramafic Ni sulfides contain high MgO and create a high melting point for the established smelting technique, thus not being processed. The feasibility of extracting Ni from this sulfide has been validated. Now efforts are underway to optimize the heat treatment for high Ni grade and large FeNi grain size.

Semiconductor assisted photocatalysis for CO2 reduction to liquid solar fuels

Yimin Wu

University of Waterloo

Abstract:

Development of sustainable and clean sources of energy, and mitigation of greenhouse gas emissions such as CO2, is among the greatest challenges facing our planet. Recently, electroreduction of CO2 has attracted considerable interest for removal of gaseous CO2. However, it is associated with significant losses primarily due to a large overpotential and electrical energy input. In addition, the use of electricity as a secondary form of energy is inefficient due to significant losses associated with conversion from primary sources to chemical fuels. Solar energy is the largest primary energy source available. Photocatalytic reduction of CO2 using solar energy offers an efficient way to convert solar energy into chemical energy and directly store it in the form of chemical fuels. Particular interest is its conversion directly into liquid fuels such as methanol. We will present CO2 reduction in a metal oxide system, namely Cu2O. It is very promising as photocatalysts with good mutlielectron transfer properties due to its loosely bonded d electrons. It is inexpensive materials with near ideal electronic properties for light energy conversion into fuels. Cu2O shows intrinsic p type conductivity due to presence of negative charged Cu vacancies with one of the lowest electron affinities, identifying Cu2O as an optimal candidate for reduction of CO2. Here, we present atomic level understanding of active sites in Cu2O that leads to the discovery of the facet specific adsorption and subsequent light induced of CO2 exclusively into liquid fuel-methanol. The activity of these active sites was unraveled using operando multimodal correlative scanning fluorescence x-ray microscopy and environmental transmission electron microscopy at atmospheric pressure, in operando, on a single particle level, we design nanoparticles with high active facet selective active sites and particles activity.

Steric Hindrance- and Work Function-Promoted High Performance for Electrochemical CO Methanation on Antisite Defects of MoS2 and WS2

Xue Yao

University of Toronto

Abstract:

CO methanation from electrochemical CO reduction reaction (CORR) is significant for sustainable environment and energy, but electrocatalysts with excellent selectivity and activity are still lacking. Selectivity is sensitive to the structure of active sites, and activity can be tailored by work function. Moreover, intrinsic active sites usually possess relatively high concentration compared to artificial ones. Here, antisite defects MoS2 and WS2, intrinsic atomic defects of MoS2 and WS2 with a transition metal atom substituting a S2 column, are investigated for CORR by density functional theory calculations. The steric hindrance from the special bowl structure of MoS2 and WS2 ensures good selectivity towards CO methanation. Coordination environment variation of the active sites, the under-coordinated Mo or W atoms, effectively lowers the work function, making MoS2 and WS2 highly active for CO methanation with the required potential of -0.47 and -0.49 V vs. reversible hydrogen electrode, respectively. Moreover, high concentration of active sites and minimal structural deformation during the catalytic process of MoS2 and WS2 enhance their attraction for future commercial application.

Systematic Study of Electrochemical Urea Synthesis from Carbon Dioxide on Metal Surfaces

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Abstract:

Extensive use of fossil fuels emits a huge amount of carbon dioxide (CO2) into the atmosphere leading to enhanced global warming and climate change. The urgency of reducing atmospheric CO2 and the profitable market breed one attractive research direction in electrocatalysis: electrochemical reduction of atmospheric CO2 (CO2RR) into valuable products. The mechanism for C-H and C-C bond formation has been widely studied on various materials and current research focuses on the industrialization of major CO2RR products.

However, the C-N bond formation in electrochemical CO2 reduction has not been well explored. One attractive C-N coupled product is urea with a relatively large market size and high market price. Electrochemical urea synthesis could be an alternative to replace current energy-intensive urea production (a two-step process from nitrogen gas with >2% global energy consumption). Here, we demonstrate pure metals exhibit high selectivity towards urea in CO2RR. And we study the electrochemical reduction of CO2 and NOx to urea systematically including pH, NOx concentration, and voltage. We find that previous knowledge from CO2RR field can be carried over to C-N formation and could further improve the efficiency of electrochemical urea synthesis.

We observe the balance between CO2 and NOx is the key factor to determine urea selectivity. With a low NOx ratio, CO2RR products dominate the energy consumption at low current density. With a high NOx ratio, NOx reduction products (such as nitrogen gas, ammonium) consume a large portion of electrons. Thus, the proper ratio of CO2 to NOx is crucial for high urea selectivity. Our study reveals the hidden mechanisms for urea electrochemical synthesis and finds the rate-determining step. The new urea synthesis could replace our current energy-intensive urea production methods.

Posters:

CO2 mitigation using Sustainable Aviation Fuels

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Abstract:

It has been clear for decades that the earth's climate is transforming. Communities and ecosystems in Canada and around the world are being affected. The extent of future warming the earth will encounter depends on how much carbon dioxide and other greenhouse gases we discharge in coming decades. According to the UN, the concentration of Green House gases (GHGs)in the earth's atmosphere is directly correlated to the average global temperature on earth. The most abundant GHG, about two-thirds, carbon dioxide (CO2), is largely the consequence of burning fossil fuels. As of 2019, The transportation division generates the greatest share of greenhouse gas emissions, about 29 percent.

Air travel is becoming one of the most used modes of travel. According to International Civil Aviation Organization (ICAO), the compilation of annual global statistics, the total number of passengers carried on scheduled services increased to a whopping 4.5 billion in 2019, while the number of departures reached 38.3 million in 2019. This means there has been a drastic increase in the emissions released by the aerospace industry as the industry uses petroleum-based fuels.

ICAO called for a significant proportion of sustainable aviation fuel (SAF) use by 2050. This paper focuses on a detailed study of sustainable aviation fuels and to study the European union assistance project which aims to contribute to the mitigation of carbon dioxide emissions from international aviation by executing capacity building activities that will back the development of low carbon air transport and environmental sustainability.