May 22-25
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Edmonton, Alberta, Canada
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Department of Mechanical, Material, and Aerospace Engineering
ORGANIZATION

Conference Chairs

LIU, Jing                                          HENEIN, Hani
University of Alberta                        University of Alberta

Local Organizing Committee

HOGAN, James                                          LI, Leijun                                          LI, Ge                                          WANG, Xiaolei
Sponsor Chair                                     Workshop Chair                                     Program Chair                                     Program Chair
MESSAGE FROM THE CHAIRS

Greetings,

We extend a warm welcome to CMSC 2024, a gathering poised to unite experts, researchers, and industry leaders in exploring the forefront of materials science. Themed "Materials Revolution: Path to Carbon Neutrality," this conference stands out for its focus on graduate student research and the celebration of Canadian excellence in materials science and engineering.

What sets CMSC 2024 apart is its diverse array of symposia, workshops, and networking opportunities meticulously crafted to foster collaboration and knowledge exchange. This dynamic environment promises to ignite creativity, fuel innovation, and pave the way for transformative solutions in materials science. Attendees can anticipate invaluable insights into cutting-edge research, emerging trends, and best practices. Whether seasoned professionals, budding researchers, or students, CMSC 2024 offers a platform to broaden knowledge, forge meaningful connections, and uncover new collaborative prospects.

To those embarking on their first CMSC journey, we urge full immersion in every learning and networking avenue. Embrace the diversity of symposia and workshops to expand horizons and explore new research avenues. Engage openly with peers, ask questions, and share experiences. Remember, CMSC transcends mere conference status—it's a catalyst for personal and professional growth, fostering collaboration and development.

Our vision is for attendees to depart CMSC 2024 not only inspired and empowered to effect change but also enriched by the warmth and camaraderie of the Alberta community. This blend of knowledge exchange and genuine connection creates an experience that transcends boundaries, leaving an indelible mark on all who participate.

Warm regards,

Conference Chairs
CMSC 2024
Ke Lu received BS in MSE from Nanjing University of Science & Technology in 1985 and PhD in MSE from Institute of Metal Research (CAS) in 1990. He served as the director of Institute of Metal Research of CAS during 2001-2012, and the founding director of Shenyang National Laboratory for Materials Science (SYNL) during 2000-2023. Currently, he is the President of Liaoning Academy of Materials, and a research professor at the Institute of metal research of CAS.

His research interests are nanostructured metals and alloys. His identity accomplishments include: (i) Discovery of nano-twinned structures and nano-twin strengthening in metals and alloys that exhibit superior combinational mechanical properties and novel physical properties, and (ii) Development of surface nanocrystallization technology for generating gradient nanostructured metals and alloys, advancing properties and performance such as fatigue behavior, wear and corrosion resistance, and surface alloying kinetics for engineering materials. (iii) Discovery of a new metastable polycrystalline structure at the extremely fine scale: Schwarz crystal structure, in which grain boundaries form 3D periodical minimal surface structure.

Prof. Lu authored and co-authored more than 430 international peer-reviewed journal publications and held 40 patents. He received many international honors and awards, including an elected member of the Chinese Academy of Sciences (2003), the World Academy of Sciences for Developing Countries (2004), the German National Academy of Sciences Leopoldina (2005), and the U.S National Academy of Engineering (2018). He is a recipient of TMS Robert Franklin Mehl Award (2022), Acta Materialia Gold Medal (2019), TMS Fellow Award (2017), AAAS Fellow (2014), MRS Fellow (2010), AvH Research Award (Germany, 2010), Kelly Lecturer (University of Cambridge, 2010), THERMEC 2006 Distinguished Award, the Third World Academy of Science TWNSO Technology Prize (2000), Ho-Leung-Ho-Lee Technology Science Prize (1999), etc.
AWARD RECIPIENTS

Keynote Speaker & The Metal Physics Award Lecturer

Dongyang Li is a Professor of Materials Science and Engineering at University of Alberta. He received a B.Sc. in Solid Mechanics from University of Science and Technology China (1982), a M.Sc. in Condensed–Matter Physics from Sun Yat-sen University (1985), a PhD in Materials Physics from University of Science and Technology Beijing (1990), and a PhD in Metallurgical Engineering from McGill University (1995). Dr. Li was a postdoctoral fellow at the Pennsylvania State University before joining the University of Alberta in 1998. He is an Adjunct Professor of Biomedical Engineering at the University of Alberta, and holds adjunct professorship at several foreign universities. Dr. Li is on the editorial board for eighteen international journals. He has more than 480 scientific publications, including more than 430 journal publications. Dr. Li is an invited contributor for authoritative handbooks on wear and tribology (Elsevier, Springer, and ASM International). He is a Fellow of the Canadian Academy of Engineering (FCAE), Member of European Academy of Sciences and Arts (MEASA), Fellow of the Institute of Materials, Minerals and Mining ((FMMM), and Fellow of the Institute of Physics (FInstP, UK). Dr. Li is the recipient of MatSoc Distinguished Materials Scientist award (2020) and other honorary titles. His interests of research include materials design, surfaces and interfaces, wear and corrosion-wear synergy, and computational materials science.

Keynote Speaker & The Metal Chemistry Award Lecturer

Edouard Asselin is a Professor at The University of British Columbia (UBC) in the Department of Materials Engineering. Since 2007, he has worked with the UBC Industrial Research Chair in Hydrometallurgy. He is also co-director of UBC’s Pipeline Integrity Institute. Dr. Asselin is an applied electrochemist: he teaches and conducts research in aqueous metal extraction, electro-metallurgy, corrosion, and protective coatings. He was the President of the Metallurgical Society of Canada in 2019, and he was a member of its Board of Directors from 2009 to 2021. Dr. Asselin has published over 150 peer-reviewed journal articles and over 40 conference publications. He is a co-inventor of two licensed and commercial technologies: the Jetti copper leaching process and a high temperature sensing platform for pressure leaching autoclaves.
Workshops

May 22, 2024

Workshop I: Computer Vision-Guided Deep Learning for Materials Science and Engineering
Length/Agenda: 9:00 am-12:00 pm with coffee/tea breaks.
Speakers and their Affiliations: Dr. Kasra Rezasefat (University of Alberta), Dr. Milad Nazarahari (Assistant Prof. University of Alberta), and Dr. James Hogan (Associate Prof. University of Alberta)
Location: ECERF-W2-050

Workshop II: Preparing for Academic Job Applications for New Graduates
Length/Agenda: 1:30 pm-4:00 pm total with coffee/tea breaks.
Speakers and their Affiliations: Dr. James Hogan (Associate Prof. University of Alberta)
Location: ECERF-W2-050

Workshop III: Advanced Material Characterization: 2D, 3D, and In-situ Microscopy and Spectroscopy (XRD, FIB/SEM and XRM)
Length/Agenda:
9:15am-12:00pm: presentations (3 talks)
12:00pm-1:30pm: Lunch (provided by nanoFAB and sponsors to registered attendees)
1:30pm-4:00pm: Hands-on demonstrations (nanoFAB facility at CME labs). Three demos are running in parallel. Attendees are required to select one. Space of each demo is limited.
Workshop Coordinators: Peng Li (Peng.Li@ualberta.ca), Nas Yousefi (nastara1@ualberta.ca), and Griselda Sukmoro (sukmoro@ualberta.ca)
Location: ECERF W2-090

More Details: https://cmscconf.org/2024-workshops/
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Symposium Title</th>
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<tr>
<td>AFTP</td>
<td>Advanced Functional Textiles and Polymers</td>
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<tr>
<td>AMSE</td>
<td>Advanced Materials for Sustainable Energy and Carbon Management</td>
</tr>
<tr>
<td>ARMB</td>
<td>Advances in Rechargeable Metal Batteries</td>
</tr>
<tr>
<td>CPCE</td>
<td>Critical Minerals: Powering Clean Energy Transitions</td>
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<tr>
<td>MCMS</td>
<td>Materials and Corrosion Management for a Sustainable Future</td>
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<tr>
<td>MACC</td>
<td>Metallic and Ceramic Coatings</td>
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<tr>
<td>MAMP</td>
<td>Metal-Additive-Manufacturing: Processing, Structure, and Properties</td>
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<tr>
<td>CSAE</td>
<td>Challenges in the Shift to Alternative Energy Futures</td>
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<td>NAHE</td>
<td>Nanomaterials Advancing the Hydrogen Economy</td>
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<tr>
<td>OMCC</td>
<td>Operando Materials Characterization for Clean Energy</td>
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Room 1: ETLC E6-060
Room 2: ETLC E2-E100 East
Room 3: ETLC E6-068/064
Room 4: ECERF W2-010
Room 5: ECERF W2-050
Room 6: ECERF W2-090/110
## AGENDA

### May 23, 2024 (Thursday)

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<td>08:30am - 09:30am</td>
<td>Registrations and Breakfast</td>
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<tr>
<td>S1</td>
<td>09:00am - 09:10am</td>
<td>Conference Welcome (By CMSC chair, ETLC E2-E100)</td>
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<td></td>
<td>09:10am - 10:10am</td>
<td>Plenary Lecture</td>
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<tr>
<td></td>
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<td>Ke Lu, Chinese Academy of Sciences</td>
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<td></td>
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<td>D.K.C. MacDonald Memorial Lecture</td>
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<td>(ETLC E2-E100, introduced by CMSC chair)</td>
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### AM

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<td></td>
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### O1

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<td>06:00pm - 08:30pm</td>
<td>Banquet Dinner (University Club)</td>
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### Notes
- S1: Session ID
- AM: AM Session
- PM: PM Session
- Coffee Break
- Lunch
### May 24, 2024 (Friday)

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<td>S3</td>
<td>09:00am - 09:45am</td>
<td>Keynote Lecture Edouard Asselin, The University of British Columbia CMSC Metal Chemistry Award Lecture (ETLC E2-E100, introduced by CMSC chair)</td>
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| O2 | 05:00pm - 06:00pm | Poster Session (ETLC E2-E100 West) |

### May 25, 2024 (Saturday)

**A One Day Round Trip to Jasper**

*Trip Lead: Mark Cui (jiayao1@ualberta.ca)*

(Itinerary on page 25)
Symposium:
Advanced Functional Textiles and Polymers (AFTP)
Thursday-Friday, May 23-24, 2024
Room: E6-060, ETLC
Chairs: Patricia Dolez, Dan Sameoto

10:20am - 10:40am, May 23
AFTP1: (Invited) Regulating Pulsatile Flows in Mock Ex-Vivo Heart Perfusion Device by Jacketed Elastomeric Tubes
Hyun-Joong Chung, University of Alberta

10:40am - 11:00am, May 23
AFTP2: Integrating Porous Materials with Phase-Change Materials for Sustainable Energy Storage and Remediation of Heavy Oil Spills
Yihao Guan, University of Alberta

11:00am - 11:20am, May 23
AFTP3: Highly Stretchable Transparent Anti-icing Self-Cleaning Shield
Jueun Lee, University of Alberta

11:40am - 12:00pm, May 23
AFTP 4: Fitting female firefighters: How alterations can enhance the safety and comfort of protective clothing
Jemma Forgie, University of Alberta

12:00pm - 12:20pm, May 23
AFTP 5: Effects of Compression and Moisture on the Thermal Insulation of Sleeping Bags
Parian Mohamadi, University of Montreal

12:20pm - 12:40pm, May 23
AFTP 6: Hydrothermal aging of PBO fabric – Effect of liquid/vapor water phase and temperature
Rajitha Botheju, University of Alberta

02:40pm - 03:00pm, May 23
AFTP 7: Additively Manufactured Colorimetric pH Sensor Based on Polyacrylamide/Alginate Double Network Hydrogels
Rayan Basodan, University of Alberta

03:00pm - 03:20pm, May 23
AFTP 8: Ushering the potential of commercial conductive textiles to be used in wearable devices to monitor health
Moshtiq-Us-Saleheen Chowdhury, University of Calgary

03:20pm - 03:40pm, May 23
AFTP 9: Fabrication of Visible Light Sensitive Electrospun TiO$_2$ Nanofibers Using Squaric Acid for Photocatalytic Application
Eba Mala Maldaye, Jimma University

04:00pm - 04:20pm, May 23
AFTP 10: Macro-texturing fabric to modify rain droplet contact time
Nicole Furtak, University of Toronto

04:20pm - 04:40pm, May 23
AFTP 11: Development and Testing of a Clear Stretchable Film for Anti-icing Applications
David Liu, University of Alberta

04:40pm - 05:00pm, May 23
AFTP12: Metamaterial Structures to Control Infrared Radiation on Polymeric Surfaces: Innovations in Radiative Thermal Management
Shima Jalali, University of Alberta

05:00pm - 05:20pm, May 23
AFTP13: Laser-assisted reduction of graphene oxide coated on melamine sponge for advanced application in electromagnetic interference shielding
Henok Atinkut Baye, Myongji University

10:00am - 10:20am, May 24
AFTP14: Development of Methods to Evaluate In-Use Firefighters’ Protective Clothing and Predict Its Remaining Service Life
David Torvi, University of Saskatchewan

10:20am - 10:40am, May 24
AFTP15: A Tiered Approach Towards Optimization of Lyocell Prototype Development
Lelia Lawson, University of Alberta
10:40am - 11:00am, May 24

AFTP16: Effect of Microclimate Thickness and Orientation, and Airflow Direction and Velocity on the Dry Thermal Resistance of Sportswear Fabrics
Md Rashedul Islam, University of Alberta

11:20am - 11:40am, May 24

AFTP17: Additive manufacturing of polyether ether ketone (PEEK)/ lunar regolith composites through fused filament fabrication
Mohammad Azami, Concordia University

11:40am - 12:00pm, May 24

AFTP18: Dynamic behavior of cross-ply fiber reinforced polymer composites under in-plane compression
Yogesh Kumar, University of Alberta

12:00pm - 12:20pm, May 24

AFTP19: Load bearing capacity and operational effectiveness of Single Shear Joints of CFRP Composite Laminate with Spread Tow Thin Plies
Tabrej Khan, Prince Sultan University

01:40pm - 02:00pm, May 24

AFTP20: Developing a Platform for the Optimization and Quality Control Management of a Perfusion Cannula Fabrication Process
Anthony Demong, University of Calgary

02:00pm - 02:20pm, May 24

AFTP21: Fabrication of Durable and Inextensible Silicon Rubber Molds Tailored for high-Pressure Embossing of IR Transparent Materials
Abolfazl Vaheb, University of Alberta

02:20pm - 02:40pm, May 24

AFTP22: Curvy mechanical metamaterials for fracture resistance, energy absorption, and vibration isolation applications
Ramin Hamzehei, University of Manitoba

02:40pm - 03:00pm, May 24

AFTP23: Organogel Coatings to Shed off Mud/Ice/Slush Contaminants
Zhitong Lin, University of Alberta

03:20pm - 03:40pm, May 24

AFTP24: An endeavor to develop a novel analysis approach for characterizing the time-dependent behavior of PE pipes
Furui Shi, University of Alberta

03:40pm - 04:00pm, May 24

Melese Shiferaw, Bahir Dar Institute of Technology - Bahir Dar University

Symposium:

Advanced Materials for Sustainable Energy and Carbon Management (AMSE)
Thursday-Friday, May 23-24, 2024
Room: E2-E100 East, ETLC
Chairs: Shiva Mohajernia, Mohd Adnan Khan

10:20am - 10:40am, May 23

AMSE1: (Invited) Design of Stable Nanocrystalline Multicomponent Alloys Towards Carbon Emission Reduction
Ahmed Tiamiyu, University of Calgary

10:40am - 11:00am, May 23

AMSE2: Solid Removal in the Warm Lime Softening Process of SAGD Water Treatment: Effects of Coagulant and Flocculant
Siyu Li, University of Alberta

11:00am - 11:20am, May 23

AMSE3: Tailoring Cu valence states in co-catalysts on ZnTe/ZnO photocathodes for syngas production
Yi-Cheng Wang, University of Alberta

11:40am - 12:00pm, May 23

AMSE4: (Invited) Challenges and prospects for the application of AI tools for the design and optimization of green energy materials
Chandra Veer Singh, University of Toronto

12:00pm - 12:20pm, May 23

AMSE5: Mesoporous BiVO4-based Photoelectrode in Water Splitting Photoreactor
Ali Tavazohi, University of Alberta
12:20pm - 12:40pm, May 23

AMSE6: Nanoindentation studies of halide perovskites

Ruitian Chen, University of Toronto

2:40pm - 3:00pm, May 23

AMSE7: (Invited) Quantifying opportunities and challenges of disruptive processes for future production of zero-CO2 ferroalloys

Sami Meddeb, Eramet Ideas

3:00pm - 3:20pm, May 23

AMSE8: Mechanism on mechanical degradation and microstructure evolution of a Cr-Mo steel over long-term service

Zhe Lyu, University of Alberta

3:20pm - 3:40pm, May 23

AMSE9: Orientation-dependence of Incipient plasticity in Mg-Gd alloy by nanoindentation

Moein Imani Fouman, University of Manitoba

4:00pm - 4:20pm, May 23

AMSE10: (Invited) Synthesis and Evaluation of Nanostructured High-Entropy Alloy Films as Advanced Catalysts for Water Splitting

Daniela Arango, Natural Resources Canada

4:20pm - 4:40pm, May 23

AMSE11: Synthesis and Evaluation of Nanostructured High-Entropy Alloy Films as Advanced Catalysts for Water Splitting

Amir Hossein Taghvaei, Queen’s University

4:40pm - 5:00pm, May 23

AMSE12: Electrochemical CO₂ fixation and conversion to green urea

Sourav Paul, Ramakrishna Mission Vidyamandira

5:00pm - 5:20pm, May 23

AMSE13: Acid–base chemistry and the economic implication of electrocatalytic carboxylate production in alkaline electrolytes

Mohammad Arshad Muzibur, University of Alberta

10:00am - 10:20am, May 24

AMSE14: (Invited) Structural Design and Electrochemical Potassium Storage Properties of Metal Chalcogenides

Yuhan Wu, Shenyang University of Technology

10:20am - 10:40am, May 24

AMSE15: Chalcogenide nanoparticle sensitized TiO₂ nanotube arrays for photocatalysis and photoelectrochemistry

Damini Vrushabendral, University of Alberta

10:40am - 11:00am, May 24

AMSE16: Effect of T4 and T6 Heat Treatment on the Microstructure and Conductivity of the Aluminum Alloy A356

Kyle Lessowayl, The University of British Columbia, Okanagan

11:20am - 11:40am, May 24

AMSE17: (Invited) Self-extinguishing solid polymer electrolytes for solid-state lithium metal batteries

Yuhang Zhang, Shenyang University of Technology

11:40am - 12:00am, May 24

AMSE18: Semi-metallic intrinsically decorated Ti-based oxide electrodes for electrochemical hydrogen generation

Ula Suliman, University of Alberta

12:00pm - 12:20pm, May 24

AMSE19: Semi-metallic intrinsically decorated Ti-based oxide electrodes for electrochemical hydrogen generation

Navneet Kumar, University of Alberta

1:40pm - 2:00pm, May 24

AMSE20: Data-Driven Design of Multifunctional Ceramic Components for Hydrogen Energy Applications

Kasra Rezasefat, University of Alberta

2:00pm - 2:20pm, May 24

AMSE21: Innovative Ni-Fe Whiskers for Highly Efficient Oxygen Evolution in Alkaline Media

Mohsen Fakourihasar, University of Alberta

2:20pm - 2:40pm, May 24

AMSE22: Nanoengineered Zn-modified Nickel Sulfide (NiS) as a Bifunctional Electrocatalyst for Overall Water Splitting

Chandra Prakash, University of Alberta

2:40pm - 3:00pm, May 24
AMSE23: Novel Polyether Block Amide Polymers for Membrane-Assisted Decarbonization
Arash Mollahosseini, Nanotechnology Research Centre, National Research Council Canada

03:20pm - 03:40pm, May 24

AMSE24: Titanate photocatalyst/polyurethane foam composite for facile biohydrogen production via photo fermentation from corn
Alemu Getu Menegeste, Myongji University

Symposium:
Advances in Rechargeable Metal Batteries (ARMB)
Friday, May 24, 2024
Room: W2-090/110, ECERF
Chair: Zhixiao Xu

10:00am - 10:20am, May 24
ARMB1: (Invited) Impact of Pressure Distribution and Magnitude on the Performance of Lithium Metal Anodes
Matthew Li, Argonne National Laboratory

10:20am - 10:40am, May 24
ARMB2: Viscoplasticity-Driven Suppression of Lithium Dendrite Penetration in Sulfide Electrolytes
Changmin Shi, Brown University

10:40am - 11:00am, May 24
ARMB3: 3D X-ray Computed Tomography Study of Si-C Composite Anodes in Li-ion Batteries
Moin Abid, McMaster University

11:20am - 11:40am, May 24
ARMB4: (Invited) Beyond Lithium: Navigating the Landscape of Sodium-ion Batteries with a Spotlight on Nanode’s Breakthroughs
Jiankuan Li, Nanode Battery Technologies

11:40am - 12:00pm, May 24
ARMB5: Challenges in Zn-Air Battery Cell Design
Matthew Labbe, University of Alberta

12:00pm - 12:20pm, May 24
ARMB6: Quantum Mechanical Investigation of Polypyrrole-MXene Nanocomposite as an Electrode Material for Magnesium-Ion Batteries
Anthony Ezika, Tshwane University of Technology

01:40pm - 02:00pm, May 24
ARMB7: (Invited) Development of High-Performance Inorganic Solid-State Battery Cathodes
Sixu Deng, Concordia University

02:00pm - 02:20pm, May 24
ARMB8: Organic-Pigment-Mediated Sulfide Electrolyte Redox for All-Solid-State Lithium–Organic Batteries with High Areal Capacity
Qihang Yu, Concordia University

02:20pm - 02:40pm, May 24
ARMB9: Self-healing and Polar Synergistic Multi-Functional Coating of Sulfur Cathodes for High-Performance Li-S Batteries
Zhao Yang, Concordia University

02:40pm - 03:00pm, May 24
ARMB10: Blocking Li Metal Dendrites with Piezoelectric Solid Polymer Electrolytes Through Coupled Piezoelectricity, Mechanics, and Electrochemistry Effects
Changmin Shi, Brown University

03:20pm - 03:40pm, May 24
ARMB11: Functional Electrolyte Additives for Zinc-Ion Batteries
Jiayao Cui, University of Alberta

03:40pm - 04:00pm, May 24
ARMB12: High performance CuHCF/Zn battery enabled by inner Helmholtz layer regulating co-solvent strategy
Ziwei Chai, University of Alberta

04:00pm - 04:20pm, May 24
ARMB13: Novel polymer separator for zinc-ion batteries
Carolina Rodriguez Baez, University of Alberta

04:20pm - 04:40pm, May 24
ARMB14: Surface Electroactive Sites of Tungstated Zirconia Catalysts for Vanadium Redox Flow Batteries
Aknachew Mebreku Demeku, National Taiwan University of Science and Technology
10:20am - 10:50am, May 23

CPCE1: (Invited) Case Studies on Reducing CRM Dependency in Canadian Industries

Patrick Flood, InnoTech Alberta

10:50am - 11:10am, May 23

CPCE2: Magnesium Doping for Enhanced Stability of Lithium Manganese Oxide Ion-sieves for Lithium Recovery from Flowback and Produced Water

Fangshuai Wu, University of Alberta

11:10am - 11:30am, May 23

CPCE3: Evaluating the Mechanical performance of High-Frequency Induction Welded TRIP 690 (AHSS) tubes with Oxide inclusions

Sydney Okoaroha, University of Waterloo

11:40am - 12:00pm, May 23

CPCE4: Crashworthiness of critical mineral-based high-entropy alloys designed for structural applications

Muyideen Adegbite, University of Calgary

12:00pm - 12:20pm, May 23

CPCE5: A Hybrid Rate Theory Model of Radiation-Induced Growth Including the Formation of Prismatic Vacancy Loops

Mahdi Mohsini, Queen’s University

12:20pm - 12:40pm, May 23

CPCE6: Oxidative Chalcopyrite Leaching under Light Effects

Binghui Li, The University of British Columbia

2:40pm - 3:10pm, May 23

CPCE7: (Invited) Industrial Scale Challenges to the Production of Battery-Grade Graphite to Meet the Exploding Demands of Electric Vehicles

Kamal Adham, Hatch Associates

3:10pm - 3:40pm, May 23

CPCE8: Improved Direct Lithium Extraction (DLE) Adsorbents for Lithium Extraction from Lithium Bearing Waters (LBWs)

Karthik Ramachandran Shivakumar, University of Alberta

4:00pm - 4:30pm, May 23

CPCE10: (Invited) Nanoscale Transport during Liquid Film Thinning Inhibits Bubble Coalescing Behavior in Electrolyte Solutions

Qingxia Liu, University of Alberta

4:30pm - 5:00pm, May 23

CPCE11: Influence of Metal-Ion Doping on Calcite Growth

Li Yue, University of Alberta

Symposium:

Materials and Corrosion Management for a Sustainable Future (MCMS)

Thursday-Friday, May 23-24, 2024

Room: E6-068/064, ETLC

Chairs: Monica Hernandez, Erick Anaya

10:20am - 10:40am, May 23

MCMS1: (Invited) Materials and Corrosion Management for a Sustainable Future

Monica Hernandez, Infinity Growth

10:40am - 11:00am, May 23

MCMS2: Effect of Hydrogen Absorption on Microstructural, Mechanical and Corrosion Properties of Aged Legacy Pipelines

Akhilesh Reddy Chopra, The University of British Columbia

11:00am - 11:20am, May 23

MCMS3: Fracture toughness mechanism in girth welded X70 pipeline steel with different Ti/N ratio

Vanda Milani, University of Alberta

11:40am - 12:00pm, May 23

MCMS4: (Invited) Investigating the behaviour of welded joints in a high toughness naval steel under different strain conditions

Alison Mark, Defence Research and Development Canada
12:00pm - 12:20pm, May 23
MCMS5: Effect of electrochemical hydrogen-charging conditions on nanomechanical properties of X80 pipeline steel
Qing Hu, University of Calgary

12:20pm - 12:40pm, May 23
MCMS6: Corrosion management of Bunsen reaction for sustainable hydrogen production from H2S splitting cycle and S-I water splitting cycle
Xiaoling Li, University of Saskatchewan

2:40pm - 3:00pm, May 23
MCMS7: Investigating Mechanical Properties of ARMOX 500T in High Strain Rates Using Direct Impact Hopkinson Pressure Bar: A Computational Study
Mohammad Mahdi Ghadiri, York University

3:00pm - 3:20pm, May 23
MCMS 8: Machine Learning Applications for Predicting Corrosion in Extreme Environments
Emily Seto, University of Alberta

3:20pm - 3:40pm, May 23
MCMS9: An Interatomic Potential for Sodium and Chlorine in both Neutral and Ionic States
Hao Sun, Queen’s University

4:00pm - 4:20pm, May 23
MCMS10: Hydrogen embrittlement susceptibility assessment of quenched and tempered casing steel
Xu Zheng, McGill University

4:20pm - 4:40pm, May 23
MCMS11: Dissociative adsorption of hydrogen molecules at Al2O3 inclusion in steels and its implication on gaseous hydrogen embrittlement of pipelines
Yinghao Sun, University of Calgary

4:40pm - 5:00pm, May 23
MCMS12: The effect of Ti/N ratio on the microstructure of the inter-critically reheated heat affected zone for a multi-pass X70 steel girth weld
Vanda Milani, University of Alberta

10:00am - 10:20pm, May 24
MCMS14: Development of CoCrNi Medium Entropy Alloy Against Hydrogen Embrittlement
Hanieh Ahmadi, University of Alberta

10:20am - 10:40am, May 24
MCMS15: Pin-on-disc wear behaviours of CoCrNi and FeCoNi medium-entropy alloys up to 1000 °C
Wandong Wang, University of Toronto

10:40pm – 11:00am, May 24
MCMS16: Interfacial Segregation and Adhesion Effects in Equiatomic CoCrFeNi High Entropy Alloy
Dennis Boakye, University of Manitoba

Symposium:
Metallic and Ceramic Coatings: Innovations, Applications, and Performance (MACC)
Friday, May 24, 2024
Room: W2-010, ECERF
Chairs: Mostafa Yakout, Maria Ophelia Jarligo, Meifeng Li

10:00am - 10:20am, May 24
MACC1: Effect of PH and Stirring Rate on Micro-Indentation Hardness and Microstructure of Ni-SiO2 Nanocomposite Coatings Electrodeposited from Deep Eutectic Solvent
Mehry Fattah, York University

10:20am - 10:40am, May 24
MACC2: Step load nanoindentation: physical model and comparative study on FCC systems
Lizhong Lang, University of Toronto

10:40am - 11:00am, May 24
MACC3: Mechanical Behavior of AlCoCrFeMo High-entropy Alloy under Uniaxial Tension using Molecular Dynamics Simulation
Nashit Jalal, University of Alberta

11:20am - 11:40pm, May 24
MACC4: Hardness of Cold-sprayed Stable Nanocrystalline High-Entropy Alloys Evaluated through Nanoindentation
Kasimuthumaniyan Subramanian, University of Calgary
MACC5: Effect of Al-Si coating weight on the experimental heat transfer coefficient of 22MnB5 steel during hot stamping

Ardhendu Bhattacharya, University of Waterloo

01:40pm - 02:00pm, May 24

MACC7: (Invited) Submerged-Arc Welding Overlay for impact abrasion applications

Jing Li, Trimay Wear Plate Ltd.

02:00pm - 02:20pm, May 24

MACC8: A "gene-like" parameter for material tailoring: Begin with the electron work function for multi-element carbide discovery—A first-principles study

Dong Zhang, University of Alberta

02:20pm - 02:40pm, May 24

MACC9: Cold Sprayed De-Icing Coating: Techno-Economic Assessment

Peter Menghesha, University of Alberta

02:40pm - 03:00pm, May 24

MACC10: Correlations between the radiometric properties of galvanneal coating and its phase composition and surface topology

Michiyo Kagaya, University of Waterloo

03:20pm - 03:40pm, May 24

MACC11: Cold Sprayed Al-Based High Entropy Alloy Coatings with Zirconium Dispersoids

Mohammad Aatif Qazi, University of Alberta

03:40pm - 04:00pm, May 24

MACC12: Self-stable Nanocrystalline High-Entropy Alloy for High-performance Metallic Coatings

Moses Adaan-Nyiak, University of Calgary

04:00pm - 04:20pm, May 24

MACC13: Effects of Chain Configuration and Stoichiometry on the Behavior of Boron Carbide at Elevated Temperature from First Principles Quasi-harmonic Approach

Sara Sheikhi, University of Alberta

04:20pm - 04:40pm, May 24

MACC14: Influence of processing parameters on mechanical properties of layer-cladded Inconel 718

Junfeng Yuan, China University of Mining and Technology

Symposium:

Metal-Additive-Manufacturing: Processing, Structure, and Properties (MAMP)

Friday, May 24, 2024

Room: W2-050, ECERF

Chairs: André Phillion, Daan Maijer

10:00am - 10:20am, May 24

MAMP1: (Invited) Extreme mechanics, materials, and manufacturing across scales

Yu Zou, University of Toronto

10:20am - 10:40am, May 24


Kai Kang, McMaster University

10:40am - 11:00am, May 24

MAMP3: Incorporating non-linear effects in fast semi-analytical thermal modelling of powder bed fusion

Shaun Cooke, The University of British Columbia

11:20am - 11:40am, May 24

MAMP4: Printability of a water-atomized low-carbon steel powder by laser powder bed fusion

Mazyar Ansari, Innotech Alberta

11:40am - 12:00pm, May 24

MAMP5: Micro-Spot Laser Direct Energy Deposition of 18Ni Maraging Steel

Christopher Paul, The University of British Columbia, Okanagan

12:00pm - 12:20pm, May 24

MAMP6: Investigating the wire deposition of TiC-inoculated AA7075 using L-DED and the influence of post-processing heat treatment.

Taha Waqar, University of Waterloo

01:40pm - 02:00pm, May 24
MAMP7: *(Invited)* Synchrotron Techniques and Their Applications in Additive Manufacturing  
*Feizhou He, Canadian Light Source*

*02:00pm - 02:20pm, May 24*

MAMP8: Effects of Sc Addition on Rapidly Solidified Al-10Si-0.4Sc (wt. %) Alloy  
*Akankshya Sahoo, University of Alberta*

*02:20pm - 02:40pm, May 24*

MAMP9: A Closer Examination of the Nature of Atomic Motion in the Interfacial Region of Crystals Upon Approaching Melting  
*Jiarui Zhang, University of Alberta*

*02:40pm - 03:00pm, May 24*

MAMP10: Continuous dynamic recrystallization during microindentation  
*Mina Dehghan, University of Calgary*

*03:00pm - 03:40pm, May 24*

MAMP11: Uncovering the Mechanism behind Two-Step Infiltration during Layered Wide Gap Brazing of MAR-M247 using B-containing Filler Metals  
*Coleton Parks, McMaster University*

*03:40pm - 04:00pm, May 24*

MAMP12: Enhancing Mechanical Properties of Al-Cu-Sc Alloy Lattice Structures Through Heat Treatment in Hybrid Investment Casting  
*Yifan Li, University of Alberta*

*04:00pm - 04:20pm, May 24*

MAMP13: Effect of layer orientation on the dynamic mechanical response of additively manufactured 18%Ni-M350 maraging steel-high entropy alloy hybrid armour plate  
*Timothy Odiaka, University of Saskatchewan*

*04:20pm - 04:40pm, May 24*

MAMP14: Direct Energy Deposition and Characterization of NiSi12-wt% Alloy Variants on Inconel 625 Substrate  
*Mohammad Ibrahim, University of Agder*

*04:40pm - 05:00pm, May 24 (Virtual)*

MAMP15: Engineering 3D Nanopatterning via Molecular Beam Holographic Lithography  
*Tian Tian, University of Alberta*

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**Symposium:**  
**Challenges in the Shift to Alternative Energy Futures (CSAE)**

Thursday, May 23, 2024  
Room: W2-090/110, ECERF  
Chairs: Qingyang Liu, Afroz Barnoush

*10:20am - 10:50am, May 23*

CSAE1: *(Invited)* The Role of Ce Addition on Strain Localization and the Evolution of Portevin-Le Chatelier (PLC) effect in Direct Chill Cast Al-5wt%Mg Alloy  
*Shengze Yin, Queen’s University*

*10:50am - 11:20am, May 23*

CSAE 2&3: *(Invited)* Influence of hydrogen uptake on additively manufactured and conventional austenitic stainless steels 316  
*Qingyang Liu, Hamad Bin Khalifa University*

*11:40am - 12:00pm, May 23*

CSAE4: Stable and Efficient Microbubble-Enhanced Cold Plasma Activation for Treatment of Flowing Water  
*Ziya Saedi, University of Alberta*

*12:00pm - 12:20pm, May 23*

CSAE5: Microbubble-Enhanced Cold Plasma for Recycling of Wastewater  
*Qiuyun Lu, University of Alberta*

*12:20pm - 12:40pm, May 23*

CSAE6: Exploring phase behavior and control of phase stability in fast pyrolysis oil  
*Ziting Sun, University of Alberta*

*02:40pm - 03:00pm, May 23*

CSAE7: On the effect of chemical composition on the Liquid Metal embrittlement susceptibility of advanced high strength steels  
*Fateme Abdiyan, McMaster University*

*03:00pm - 03:20pm, May 23*

CSAE8: On the Serration Characteristics, Strain Localization Patterns and Crystallographic Texture Development during Tensile Testing of
Thermomechanically Processed Thin-Strip Continuous Cast AA5182 Alloy

Hesam Pouraliakbar, Queen’s University

03:20pm - 03:40pm, May 23

CSAE9: A computationally efficient microstructure evolution model of dynamic recrystallization during hot rolling process

Shabnam Fadaei Chatroudi, McMaster University

04:00pm - 04:20pm, May 23

CSAE10: Modeling of hydrogen atom distribution at corrosion defect on existing pipelines repurposed for hydrogen transport under pressure fluctuations

Jin Zhang, University of Calgary

04:20pm - 04:40pm, May 23

CSAE11: Influence of pipeline steel microstructure on hydrogen uptake after gaseous and electrochemical charging

Tonye Jack, University of Saskatchewan

04:40pm - 05:00pm, May 23

Symposium:

Nanomaterials Advancing the Hydrogen Economy (NAHE)

Friday, May 24, 2024

Room: E6-068/064, ECERF

Chair: Karthik Shankar

01:40pm - 02:00pm, May 24

NAHE1: (Invited) Role of microstructures in hydrogen diffusion in structural metals

Jun Song, McGill University

02:00pm - 02:20pm, May 24


Narendra Chaulagain, University of Alberta

02:20pm - 02:40pm, May 24

NAHE3: Environment-friendly Cu:ZnInSe/ZnSeS core/shell QDs sensitized TiO2 photoanode for efficient photoelectrochemical hydrogen production

Kokilavani Shanmugasundaram, Institut national de la recherche scientifique

02:40pm - 03:00pm, May 24

NAHE4: Bismuth oxyhalide based photocatalysts for solar driven green H2 fuel production

Md Masud Rana, University of Alberta

03:20pm - 03:40pm, May 24

NAHE5: Catalytic Water Gasification and Carbon Reforming at ≤300 °C – It’s About Mechanism, not Structure.

Jeff Stryker, University of Alberta

03:40pm - 04:00pm, May 24

NAHE6: A combination of first-principle and thermodynamics study of hydrogen uptake on steel

Aliakbar Sheikhzadeh, University of Alberta

04:00pm - 04:20pm, May 24

NAHE7: Porous and non-porous bimetallic alloy nanoparticle photocatalysts

Harshitha Rajashekar, University of Alberta

04:20pm - 04:40pm, May 24

NAHE8: p-type carbon nitride for photocatalytic and photoelectrochemical hydrogen generation

Biya Saji, University of Alberta

04:40pm - 05:00pm, May 24

NAHE9: 1T&2H-MoS2/Ni3S2 Heterojunction Supported by Nickel Foam for overall Water Splitting

Michael Zeming Li, University of Alberta

Symposium:

Operando Materials Characterization for Clean Energy (OMCC)

Thursday, May 23, 2024

Room: ECERF W2-010

Chairs: Zhi Li, Keren Jiang

10:20am - 10:50am, May 23
OMCC1: (Invited) Microstructure Evolution of Amorphous Titanium Oxide: The Role of Environmental Transmission Electron Microscope

Jian Chen, NRC Nano

10:50am - 11:10am, May 23

OMCC2: Operando microwave characterization of carrier dynamics in photodetectors and photocatalysts

Navneet Kumar, University of Alberta

11:10am - 11:30am, May 23

OMCC3: Axial O ligand modulated Fe-N4 sites for highly efficient electrocatalytic nitrogen reduction

Yang Yang, University of Alberta

11:40am - 12:10pm, May 23

OMCC4: (Invited) nanoFAB Centre – A central hub of operando materials characterization

Xuehai Tan, University of Alberta

12:10pm - 12:30pm, May 23

OMCC5: Surface Microlenses for Enhanced Photodegradation of Organic Contaminants in Water

Qiuyun Lu, University of Alberta

12:30pm - 12:50pm, May 23

OMCC6: Rare earth Ce-modified V2O5 materials as the cathode for zinc-ion batteries

Xuesong Xie, University of Alberta

2:40pm - 3:00pm, May 23

OMCC7: (Invited) In Situ/Operando Studies of Cu Catalysts for Electrochemical CO2 Reduction by Soft X-ray Spectro-microscopic Characterization

Chunyang Zhang, McMaster University

3:00pm - 3:20pm, May 23

OMCC8: Exploring a New Approach for Porous Bioactive Glass Composites

Marzieh Matinfar, University of Alberta

3:20pm - 3:40pm, May 23

OMCC9: The Nanoindentation Response of Single Crystal Magnesium Using a Finite Element Model That Incorporates the Slip Systems

Syed Taha Khursheed, University of Manitoba

4:00pm - 4:20pm, May 23

OMCC10: (Invited) Synchrotron Techniques and Their Applications in Additive Manufacturing

Feizhou He, Canadian Light Sources

4:20pm - 4:40pm, May 23

OMCC11: Constructing highly dispersed nickel atoms in bamboo liked-carbon nanotubes for efficient oxygen reduction

Yifan Li, University of Alberta

4:40pm - 5:00pm, May 23

OMCC12: Lightweight Al3Ti-based medium-entropy alloys with well-balanced strength and ductility at room and elevated temperatures

Guijiang Diao, University of Alberta

5:00pm - 5:20pm, May 23

OMCC13: (Virtual) Advanced Characterization of Nanostructured Energy Materials

Babak Shalchi, NRCan CanmetMATERIALS
Introduction to Schwarz crystal—a novel metastable structure in extremely-fine-grained metals

Ke Lu
Chinese Academy of Sciences & Liaoning Academy of Materials

Abstract:
Most metals exist in the form of polycrystalline states consisting of crystalline grains and grain boundaries. Although with some novel properties such as much elevated hardness and strength, polycrystalline metals with nano-sized grains become unstable. Upon heating or straining, nano-sized grains tend to coarsen through grain boundary migration, or transform into metastable glassy phases when the grains are extremely small, eliminating grain boundaries in both processes. Recently, we found a different metastable structure in polycrystalline face-centered-cubic pure metals and alloys as their grains are refined to extremely-fine sizes (a few nanometers), namely “Schwarz crystal” (1,2). In this structure, the grain boundary networks evolved into the 3D periodical minimal surface (TPMS) configuration constrained with high density twin-boundaries. It is thermally so stable that grain coarsening is inhibited at temperatures even up to the melting point, and its strength is close to the theoretical value. Diffusional processes in alloys like precipitation of intermetallic phase, spinodal decomposition, as well as melting are inhibited with the Schwarz crystal structure (3,4). In this presentation, I will introduce the formation process, structure characteristics, and some properties of the Schwarz crystal structures in a number of pure metals and alloys. Perspectives and future studies on the structure will be discussed.

References:
Towards Electronic Metallurgy – An Electron Work Function Based Framework for Material and Surface/Interface Design

Dongyang Li

University of Alberta

Abstract:

With rapid technological advance and increase in industrial demand for high-performance materials, material design and surface/interface control have been required to rely on more fundamental principles. Various surface/interface and bulk properties of materials are largely governed by their electron behavior, which determines the atomic bond strength and system’s stability. Significant effort has long been made to correlate the properties to the electron state based on quantum mechanics. However, quantum theories are complicated and unfeasible for material design, especially for structural materials which consist of various phases and imperfections. It is thus highly wished to have simple but fundamental parameters, which reflect the electron behavior of materials, for material analysis and design. In this talk, electron work function (EWF), which is the minimum energy to move electrons at Fermi level inside a metal to its surface, is demonstrated to be a promising indicator carrying “genetic-like” information for analyzing materials and providing clues for guiding material design and surface/interface modification. Correlations between EWF and properties of materials and surfaces/interfaces will be analyzed, and the development of an EWF-based material design methodology or framework towards “electronic metallurgy” will be discussed.
Hydrometallurgy: the future of copper processing?

Edouard Asselin

The University of British Columbia

Abstract:

Chalcopyrite (CuFeS$_2$) is the world's most abundant copper mineral, accounting for at least 60% of global primary copper production. Copper is a necessary metal for the clean energy transition, and it is expected that this transition will require that we make more copper over the next 25 years than has been produced in the last 5,000 years. Mineral concentrates of chalcopyrite are processed almost exclusively by pyrometallurgical smelting and converting methods. However, these methods suffer from several key shortcomings. New methods to extract copper from chalcopyrite have been investigated across the globe for more than 50 years, but past processing breakthroughs have been rare and commercially unsuccessful. Recent scientific insights about the mineral/solution interface have resulted in promising new hydrometallurgical (aqueous chemistry-based) process development. The challenges and opportunities for the hydrometallurgical processing of chalcopyrite concentrates will be discussed in this presentation. An overview of ongoing work at UBC will be presented.
Preparation for the trip:
- Please check the weather in Jasper and make sure you wear proper clothing.
  - Long sleeve shirts and water-resistant jackets are recommended.
  - Comfortable shoes.
- Sun protection (e.g., sunscreen, sunglasses).
- Food/snacks and drink. This is a non-drinking trip and **NO alcohol will be allowed on-board**.
- Please follow the lead of our volunteers.
- **Please arrive on time.**

**Saturday, May 25, 2024**
5:30 am  Load bus from Hub Mall parking lot (East of Hub Mall, 112 St NW, Edmonton, AB T6G 2C5).
- **Please arrive on time. We will leave at 6:00 am sharp.**
- Waivers will need to be signed onsite.
6:00 am  Depart for Jasper National Park.
9:00 am  A quick stop may be made in Hinton at the A & W and Tim Hortons (325 Gregg Ave, Hinton, AB T7V 2A7).
10:15 am  Approximate arrival at Maligne Canyon.
  - 2.3-mile loop trail. Takes an average of 1 h 5 min to complete.
  - **Please travel in groups.** If you are travelling alone, please let the volunteers know and we can hike together!
  - We will stay for approximately 2 h to give everyone a chance to explore the trail and enjoy the view!
  - Information (FAQ) as well as views from this trail can be found at
    - [https://www.jasper.travel/maligne-canyon/#faq](https://www.jasper.travel/maligne-canyon/#faq)
12:15 pm  Depart for Maligne Lake.
1:00 pm  Approximate arrival at Maligne Lake.
  - Dining and boat rental options available (at your own cost). Please check the websites for more information.
  - Staying for 1 h 15 min at Maligne Lake.
2:15 pm  Depart for Jasper Town.
3:15 pm  Approximate arrival at Jasper Town.
  •  Shopping and dinning options available.

5:45 pm  Bus will be available for loading at the parking lot.
  •  If you are not returning to Edmonton with us. Please let our volunteers know.
  •  Public bus options may be available (e.g., Services provided by SunDog and Ebus).

6:15 pm  Bus will depart for Edmonton.
7:15 pm  Quick stop in Hinton at the A & W and Tim Hortons (325 Gregg Ave, Hinton, AB T7V 2A7).
10:30 pm  Approximate arrival in Edmonton.

Friendly reminder: Please make sure to bring any personal belongings with you. Leaving personal belongings on the bus is at your own risk.
Disclaimer: All times are approximate and subject to change.
Useful links:
https://parks.canada.ca/pn-np/ab/jasper/visit
https://parks.canada.ca/pn-np/ab/jasper/visit/depliants-brochures

Additional information
  •  Waiver form will need to be signed onsite for all participants prior to getting on the bus.
  •  Only conference attendees can purchase the trip ticket. If you would like to travel with your significant other, the same rate applies. You are allowed to bring one guest (i.e., maximum 2 trip tickets can be purchased).
  •  You do not have to return to Edmonton with us. If you would like to extend your stay in Jasper, please let us know. You are responsible for the extra expenses and trip plans (e.g., booking of accommodation and transportation). The price of this trip stays the same no matter whether you travel back with us or not.
  •  Booking is first come first serve. Book early since we only have a limited number of seats!
  •  No refunds will be issued if you arrive late for the departure from Edmonton to Jasper. Please arrive on time!
Abstract Appendix

Symposium: Advanced Functional Textiles and Polymers (AFTP)
Thursday-Friday, May 23-24, 2024
Room: E6-060, ETLC
Chairs: Patricia Dolez, Dan Sameoto

10:20 am - 10:40 am, May 23
AFTP1: (Invited) Regulating Pulsatile Flows in Mock Ex-Vivo Heart Perfusion Device by Jacketed Elastomeric Tubes
Hyun-Joong Chung, University of Alberta
Abstract: The ex vivo heart perfusion (EVHP) device allows the donor heart to maintain full functionality during transfer between extraction and implantation surgeries. One of the current challenges include the mismatches in mechanical properties of synthetic tube materials compared to human aorta. Here, we created an elastomeric tube that can self-regulate the degree of distension without the need of feedback controller. The tube was made of mold-casted silicone elastomer whereas a fabric 'jacket' is placed onto the outer surface. A hydraulic pressure testing rig with a camera was custom-built to monitor the deformation of the tube under internal hydrostatic and hydrodynamic (i.e., pulsatile flow) stress conditions. In the hydrostatic study, we found: (1) The tube's distension is regulated by the 'J-shaped' stain-stiffening of the 'jacket', and the degree of distension with respect to the material design is quantitatively predicted by our simulation with remarkable precision. (2) Highly asymmetric distension like 'aneurysm', common to elastomeric tubes due to imperfection in fabrication, is prevented dramatically by the self-regulation of the 'jacket'. (3) In ABAQUS simulation, our result evidences that the irreversible hysteresis behavior of elastomeric material must be considered in predicting the deformation of elastomeric structures under pre-existing deformation. In the hydrodynamic study, we found (4) the resulting pressure waveforms resemble physiological pressure waveforms far more closely than those produced from a rigid tube installed in the flow loop. (5) Hysteresis loops per each cycle of pulsatile flow provides an insight to assess the effect of viscoelasticity of the tube material on fluid retention behavior of the jacketed tube. In short, our study shows that the similar design principle can be a simple and effective strategy in regulating the flow of fluid therein, as well as in preventing aneurysm-like rupture of the tube.

10:40 am - 11:00 am, May 23
AFTP2: Integrating Porous Materials with Phase-Change Materials for Sustainable Energy Storage and Remediation of Heavy Oil Spills
Yihao Guan, University of Alberta
Abstract: Due to the low fluidity, safe and efficient cleanup of viscous oil spills still remain a great challenge, especially in frigid region. The viscosity of crude oil is highly sensitive to temperature, so increasing the temperature of three-dimensional porous materials (3D-PMs) has becoming a promising approach to accelerate the removal of viscous crude oil. Although the 3D-PMs can be heated in situ by electricity or sunlight irradiation, it is extremely difficult to build a large-scale conductive 3D-PMs or overcome the instability and intermittent of sunlight in practical application. In order to solve this problem, 3D-PMs coupled with phase change materials (PCMs) is innovatively proposed in this study. Through the pre-stored energy by PCMs from sunlight irradiation or electric heating, the heat can be released when the 3D-PMs are in contact with crude oil. A novel superhydrophobic melanine sponge (PPCPP@MS) composed of polypropylene (PPy) and polyethylene glycol (PEG) for photo/electric assisted energy storage is successfully designed. The PPy polymerization layer can stably convert photo/electricity to heat, and the PEG-CNT composite coating layer is used to realize the store and release of heat, which can greatly improve the safety, energy utilization efficiency and operability. After 10 cycles of crude oil adsorption process, its adsorption performance still maintained at 13 g g⁻¹. For the simulation of the marine environment with low-temperature, PPCPP@MS exhibits a stable heat release and oil-adsorbing performance, implying its great potential in dealing with oil spills in extreme marine climates. Overall, the innovative design of PPCPP@MS shows important guiding significance for dealing with viscous oil spills or in frigid region.

11:00 am - 11:20 am, May 23
AFTP3: Highly Stretchable Transparent Anti-icing Self-Cleaning Shield
Jueun Lee, University of Alberta
Abstract: In this work, we introduce an advanced organogel that represents a significant leap in anti-icing and anti-fouling capabilities beyond conventional polydimethylsiloxane (PDMS) materials, such as Sylgard. Our organogel is synthesized through hydrosilylation, employing vinyl-terminated PDMS, methylhydrodiosiloxane-PDMS copolymer, and varying concentrations of platinum catalyst. This approach enables precise control over the organogel's elasticity by adjusting the methylhydrodiosiloxane and catalyst levels. Furthermore, the incorporation of vinyl-terminated PDMS with functional groups or elements (e.g., fluorine) through hydrosilylation allows for the tailoring of its chemical and physical properties post-synthesis. Experimental comparisons highlight the organogel's exceptional ice-phobic properties relative to conventional materials like glass, steel, and Sylgard 184, as demonstrated by our custom ice-adhesion testing apparatus. This testing reveals significantly reduced ice-adhesion strength, underscoring the material's potential in mitigating ice accumulation. Moreover, the organogel maintains its transparency, enhancing its applicability in
optical applications, including protective shields for autonomous vehicle sensors. The synthesis flexibility, coupled with its unique combination of mechanical and surface properties, positions our organogel as an innovative material solution for environmental protection of sensitive equipment in adverse conditions. Its transparency and anti-icing capabilities open new avenues for application in optical and sensor technologies, particularly in environments where visibility and performance are critical.

11:40 am – 12 pm, May 23
**AFTP4**: Fitting female firefighters: How alterations can enhance the safety and comfort of protective clothing  
**Jemma Forgie**, University of Alberta  
**Abstract**: Fire protective clothing (FPC) is essential in protecting firefighters against the extreme environments they face during their daily work. However, the effectiveness of the FPC is reliant on how well it fits the wearer. Poorly fitted FPC may result in increased risks of heat stress, chemical exposure, and injuries such as slips, sprains, and falls. Female firefighters, a growing minority in the field, face significant challenges in finding well-fitted FPC. This can result in mobility, comfort, and functionality issues. To overcome these challenges, female firefighters have been reported to alter their fire protective clothing to improve fit and function. However, the impact of these alterations on the overall safety of the garments has not been determined. As a preliminary step toward understanding the role of alterations, this phase of the project focuses on collecting data from female firefighters across Alberta through surveys, interviews, and garment examinations. The data collected will help us understand what types of alterations they are performing on their garments, and how these alterations impact their experiences in the FPC. The collected data will be used to build lab-scale models of the alterations and test the safety of these new material systems using relevant textile test methods. This will provide meaningful information on how alterations can be used to improve the fit of protective clothing without compromising safety. Moving forward, these methods can be used to improve the fit of protective clothing for various marginalized groups across fields that require standardized protective clothing.

12 pm – 12:20 pm, May 23
**AFTP5**: Effects of Compression and Moisture on the Thermal Insulation of Sleeping Bags  
**Parian Mohamadi**, University of Montreal  
**Abstract**: This project aims to create a procedure for evaluating the thermal resistance of textile assemblies in sleeping bag manufacturing, considering compression and vapor transmission in humid conditions. Using a specialized test bench and anthropometric data, it will assess the effects of pressure and humidity on thermal resistance. Initially, the human participants with varying weight and height will be recruited to determine the pressure applied by different parts of the body using a mapping pressure mattress. Subsequently, samples will undergo different levels of pressure representing those exerted by a person lying down. The resulting thermal resistances will be compared to resistances measured without compression. The obtained results will facilitate assessing the impact of body pressure on the thermal insulation of sleeping bags, offering innovative perspectives for cold-weather outdoor protection equipment. These findings can directly benefit the technical textile industry in developing various types of insulating textile assemblies.

12:20 pm – 12:40 pm, May 23
**AFTP6**: Hydrothermal aging of PBO fabric – Effect of liquid/vapor water phase and temperature  
**Rajitha Botheju**, University of Alberta  
**Abstract**: Safety is one of the key aspects of firefighters’ job. To protect them from the hazards of their work, they wear bunker suits made with high-performance polymeric fibers. The fabrics display excellent performance when new; however, the high-performance polymers age over time, which may affect the performance of the fire-protective fabrics. In addition, these fabrics may suffer a major loss in performance before signs of degradation are visible to the naked eye, which further increases the safety concerns for firefighters. Poly(p-phenylene-2,6-benzobisoxazole) (PBO) is one of the high-performance polymers used to manufacture fibers for fire-protective fabrics. However, PBO fibers may be susceptible to hydrothermal aging because of polyphosphoric acid residues from the manufacturing process on their surface. The general objective of this study is to understand the impact of different hydrothermal conditions relevant to firefighting on the mechanical performance of a 100% PBO fabric after hydrothermal aging. This includes the impact of exposure to the liquid or vapor phase of water and the effect of temperature on the fabric’s hydrothermal aging behavior. Fabric specimens were subjected to hydrothermal aging either by immersing them in water or exposing them to 100% relative humidity (RH). The experiments were conducted at 21, 60, 80, and 90°C with exposure times between 10 and 50 days. The specimen residual mechanical strength was assessed following the ASTM D 5035 standard test method. According to the results obtained, temperature significantly affected the PBO fabric’s residual strength after hydrothermal aging. On the other hand, water immersion and exposure to 100% RH led to similar results in terms of tensile strength. The results of this study shed new light on the hydrothermal aging behavior of PBO fibers in conditions relevant to service and will contribute to making firefighting safer.

2:40 pm – 3 pm, May 23
**AFTP7**: Additively Manufactured Colorimetric pH Sensor Based on Polyacrylamide/Alginate Double Network Hydrogels  
**Rayan Basodan**, University of Alberta  
**Abstract**: We present an additively manufacturable, nanocomposite hydrogel that is capable of displaying the pH level of aqueous media by colour change for the application of environmental monitoring. The printing of
the hydrogels is prepared by free radical polymerization of a 3D printable custom ink of acrylamide/alginic acid, methacrylated phenol red, and laponite nano clay in the presence of an APS/TEMED initiator system. The nanocomposite tough hydrogel is composed of an acrylamide/alginic acid double network. The methacrylated phenol red is copolymerized with the acrylamide, which prevents the phenol red from leaching into the aqueous environment. The rheological modifier (Laponite) was used for the hydrogel precursor to have a high viscosity and be shear thinning, which are requirements for 3D printing. The rheology of the precursor solution was optimized and characterized so it can be extruded and hold its shape after being printed until it is polymerized in post processing. The mechanical properties and chemical composition of the hydrogel were studied. And the colorimetric pH response of the hydrogel was also demonstrated. This additively manufacturable and pH indicating hydrogel is suitable to be used in soft robotic and sensor applications for environmental monitoring of natural aqueous systems.

3 pm – 3:20 pm, May 23
AFTP8: Ushering the potential of commercial conductive textiles to be used in wearable devices to monitor health
Moshfiq Chowdhury, University of Calgary
Abstract: The growing interest in wearable biosensor technology has catalyzed research into integrating sensing capabilities seamlessly into everyday life. Among the various wearable applications for electrochemical monitoring of physiological parameters through sweat analysis, the potential of conductive textiles remains largely untapped. This research aims to bridge this gap by exploring the integration of conductive textiles into wearable biosensors, offering a novel approach to enhance flexibility and comfort for users. Through a comprehensive analysis of the electrical and electrochemical properties of conductive textiles, this research evaluates their suitability for use in bio wearable technology. The future field application of these sensors includes continuous health monitoring, stress and emotional state tracking in military personnel, and the early detection of health anomalies.

3:20 pm – 3:40 pm, May 23
AFTP9: Fabrication of Visible Light Sensitive Electrospun TiO2 Nanofibers Using Squaric Acid for Photocatalytic Application
Eba Mala Maldaye, University of Alberta
Abstract: Degradation of organic pollutants using photocatalysts has gained utmost importance, due to the increasing environmental pollution. Despite various attempts to improve the photocatalytic efficiency of well-known photocatalysts such as titanium dioxide (TiO2), by making them visible light active, various issues need to be resolved. In this work, attempts have been made to improve the visible light absorption capacities of the electrospun TiO2 nanofibers by modification using squaric acid (SqA). An interfacial charge transfer complex is formed by the condensation reaction between the hydroxyl groups on the surface of the TiO2 nanofibers and the SqA ligand. Various characterizations confirmed that the modification using SqA had led to the formation of the interfacial charge transfer layer, without affecting the crystallinity or morphology of the TiO2 nanofibers. The modified TiO2 nanofibers showed sensitivity to visible light with red shift in the optical absorption. It exhibited an improved photocatalytic efficiency of 85% against the degradation of tetracycline, compared with 60% for unmodified TiO2 nanofibers. It also showed an increased rate of degradation of 0.21 mg/L/min, when compared with the 0.13 mg/L/min of unmodified TiO2 nanofibers.

4 pm – 4:20 pm, May 23
AFTP10: Macro-texturing fabric to modify rain droplet contact time
Nicole Furtak, University of Toronto
Abstract: Flat, hard superhydrophobic surfaces have incorporated macro-texturing to change the droplet hydrodynamics and reduce the contact time of impacting droplets. This project investigated incorporating macro-texturing on superhydrophobic fabrics and the resulting changes in droplet impact behaviour and contact time. The selected fabrics were treated with silica nanoparticle spray followed by a silicone coating, attaining super hydrophobicity on the fabric with advancing and receding contact angles / = 162°/158°. A droplet impact apparatus and high-speed camera were used for characterization. Water droplets 1.47 mm in diameter were released from a height of 10 cm using a syringe pump with 22 gauge needle. Sewing techniques were used to create macro-textured features in fabrics commonly used in athletic wear. We found that peaks and valleys of the macro-textured fabrics were able to alter droplet rebound mechanics and reduce contact time, but only when the droplet impacted on a peak. The spacing of texture features was also an important consideration for creating fabrics with reduced contact time that was not heavily dependent on impact location. The differences in droplet behaviour with varying macro-texture will be discussed. This work aims to understand how macro-textured fabric can be used to reduce the contact time of impacting droplets.
reinforcing the gel with an auxetic structure, we expect to harness the advantage of biaxial stretchability for enhanced shedding of the foulants. In order to validate this idea, DIC (Digital Image Correlation) will be used to determine the effect that the curing agent/auxetic structure has on the gel by measuring displacement and strain.

4:40 pm – 5 pm, May 23

AFTP12: Metamaterial Structures to Control Infrared Radiation on Polymeric Surfaces: Innovations in Radiative Thermal Management

Shima Jalali, University of Alberta

Abstract: In this presentation, we study an innovative method to manipulate thermal infrared (IR) radiation through polymeric surfaces via metamaterial structures for radiative thermal management. It focuses on controlling absorption and scattering in both IR and visible range through micro-structuring of thermally transparent polymer sheets, primarily low-density polyethylene (LDPE) and high-density polyethylene (HDPE). Surfaces with lenticular lens and micro pillar structures on PE sheets (50-200 µm thick) are investigated to understand their optical and IR properties. The experimental manufacturing process involves using silicone molds reinforced with fiberglass metamaterials in applications like thermal camouflage and passive radiative cooling for buildings.

5 pm – 5:20 pm, May 23

AFTP13: Laser-assisted reduction of graphene oxide coated on melamine sponge for advanced application in electromagnetic interference shielding

Henok Atinkut Baye, Myongi University

Abstract: Owing to their unique porous structure and excellent mechanical properties, i.e., lightweight, flexibility, compressibility, and breathability melamine foam (MF)-based electromagnetic interference (EMI) shielding materials are an excellent choice. For applications in EMI-shielding, MFs need to be modified with conductive materials, like reduced graphene oxide (rGO). The state-of-art surface modifications of MF with rGO involves, coating GO on MF followed by reduction of GO to rGO hydrothermally in the presence of toxic and hazardous chemicals, like hydrazine. To avoid the use of such toxic chemicals, herein, we propose a facile and green laser-induced reduction process of GO coated on the surface of MF. First, GO was deposited on MF via simple dip coating. Next, the GO/MF composite was subjected to a femtosecond (fs) laser (780 nm wavelength; 70 fs pulse width; 50 MHz repetition rate) with a varied power range, 2 - 18 mW. The mechanism of reduction was studied via different analytical tools, i.e., SEM, XPS, and Raman spectroscopy. Results revealed that the laser-induced reduction of GO involves two pathways: (i) direct transformation from sp3 to sp2 carbon and (ii) cleavage and removal of oxygen functionalities. Performance evaluation of the EMI properties of the rGO/MF composite material is currently under investigation.

10:00 am - 10:20 am, May24

AFTP14: Development of Methods to Evaluate In-Use Firefighters’ Protective Clothing and Predict Its Remaining Service Life

David Torvi, University of Saskatchewan

Abstract: Firefighters are not only interested in the performance of their protective clothing when new, but also how its performance changes with time due to thermal exposures, environmental conditions (e.g., ultraviolet radiation), abrasion and other aging factors. Most standard tests used to evaluate the performance of this clothing are destructive, so there is a need to develop nondestructive tests for assessing in-use clothing, to assist fire departments in determining when an individual garment should be retired from service. This research group has investigated a number of potential nondestructive tests for firefighters’ protective clothing, the results of which can be correlated with changes to key properties of fabrics, such as tensile strength. While earlier methods were based on fabric colour measurements, research is currently focused on models that consider changes in near-infrared (NIR) spectral data.

This presentation will discuss the results of a study in which protective fabrics used in wildland and structural firefighters’ protective clothing were exposed to heat fluxes from 10 to 70 kW/m^2 for various durations using a cone calorimeter. These heat fluxes represent a wide range of firefighting conditions, from initial operations outside a building to emergency conditions for which this clothing provides an opportunity to escape. The tensile strength of a fabric specimen was measured after each exposure, along with the reflectance between 400 and 2500 nm. Fabric temperatures measured during the exposures and thermal gravimetric analysis results were used to assist in interpreting results. Examples of correlations between tensile strength and heat flux/exposure duration developed in this research will be presented. Future work to improve these correlations and NIR spectral data analysis techniques will also be discussed, along with research needed to develop practical devices to implement NIR-based methods to assess protective clothing in the field.

10:20 am - 10:40 am, May24

AFTP15: A Tiered Approach Towards Optimization of Lyocell Prototype Development

Leila Lawson, University of Alberta

Abstract: Lyocell manmade cellulose fibres (L-MMCF) are typically manufactured from wood sources and bamboo. Current sustainability trends have led to research on L-MMCF from alternative agricultural feedstocks; however, determining the viability of these feedstocks can be challenging in lab-scale settings. This presentation describes the exploration and utilization of readily available lab-scale equipment to manufacture small quantities of lyocell fibres as part of a tiered approach to optimize the L-MMCF manufacturing process. Preliminary findings of suitability are discussed for various wood, agricultural and recovered cellulose feedstocks. Qualitative physical characteristics of the spun fibres are presented, as well as a discussion
outlining how lab-scale equipment can be utilized to differentiate and characterize L-MMCF from various feedstocks. This research provides a simple, cost effective, and efficient method for analysis of various feedstocks towards L-MMCF manufacturing and their viability.

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<th>10:40 am – 11:00 am, May 24</th>
<th>AFTP16: Effect of Microclimate Thickness and Orientation, and Airflow Direction and Velocity on the Dry Thermal Resistance of Sportswear Fabrics</th>
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<td>Md Rashedul Islam, University of Alberta</td>
<td><strong>Abstract:</strong> The influence of fabric properties, garment fit, and environmental factors on human thermophysiological comfort is of interest in the sportswear industry as they contribute to the performance of athletes. The present study investigated the effect of microclimate thickness and orientation (horizontal or vertical), as well as the airflow direction (normal or parallel to the fabric surface) and velocity (1 and 10 m/s), on the dry thermal resistance in the skin-cloth-environment system using 27 sportswear fabrics. The experiments were conducted based on the ISO 11092 standard test method with modifications to the test conditions. For both microclimate orientations, the total dry thermal resistance (Rct) initially increased with increasing microclimate thickness. This increase in Rct can be associated with the reduction in the conductive heat transfer through the layer of stagnant air in the microclimate. In the case of the horizontal microclimate, the Rct values decreased above a certain microclimate thickness due to natural convection and then increased slightly again. For the vertical orientation, the Rct values plateaued after the onset of natural convection in the microclimate. With the airflow direction normal to the fabric surface, a horizontal orientation, and no air gap between the fabric and the hot plate, the Rct values were positively correlated with the fabric thickness. In the presence of a 9 mm-thick vertical microclimate with normal airflow, the Rct values were negatively correlated with the fabric air permeability. For highly permeable fabrics, the vertical airflow direction with a velocity of 10 m/s shifted the onset of natural convection in the horizontal microclimate towards a smaller microclimate thickness. The findings of this study contribute to improved fabric selection and optimization of the design process of sport garments for enhanced thermal comfort and performance of athletes.</td>
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<th>11:20 am – 11:40 am, May 24</th>
<th>AFTP17: Additive manufacturing of polyether ketone (PEEK)/lunar regolith composites through fused filament fabrication</th>
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<td>Mohammad Azami, Concordia University</td>
<td><strong>Abstract:</strong> The NASA Artemis Program is driving advancements in space settlement and exploration. In the realm of extended space exploration, in-space manufacturing (ISM) plays a vital role, with additive manufacturing (AM) showing great promise. Polyether ketone (PEEK) emerges as an ideal material for lunar environments, and the fused filament fabrication (FFF) method for 3D printing it offers distinct advantages. The integration of lunar regolith into PEEK proves to be a cost-effective strategy for ISM. This research specifically delves into the FFF of PEEK/regolith composites, comparing them with pure PEEK and PEEK infused with chopped carbon fiber. SEM micrographs demonstrate a random distribution of solid material in the matrix, proving the effective selection of the mixing strategy. The higher content of solid material poses challenges during extrusion, resulting in increased porosity in the samples. The introduction of 20 wt% carbon fiber boosts tensile strength by 8.37%, while the inclusion of 15 and 30 wt% lunar regolith diminishes tensile strength by 14.63% and 26.78%, respectively. This leads to more brittle fractures and reduced elongation at break. These findings carry significant implications for advancing additive manufacturing in lunar environments and in-space manufacturing.</td>
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<th>11:40 am – 12 pm, May 24</th>
<th>AFTP18: Dynamic behavior of cross-ply fiber reinforced polymer composites under in-plane compression</th>
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<td>Yogesh Kumar, University of Alberta</td>
<td><strong>Abstract:</strong> Laminated composites have been widely used in aerospace and defense industries owing to high specific strength and stiffness. The anisotropic nature of fiber reinforced composite necessitates in-depth understanding of effect of the ply orientation and thickness on the mechanical properties in a cured structural laminate. In addition, the strain-rate dependency and the complex failure modes of such advance materials entails characterization under dynamic loading conditions. In this study, cross-ply carbon-based fiber reinforced polymer composite laminates are experimentally evaluated under dynamic uniaxial in-plane compression. Three laminates with varied number of 90° plies (n = 4, 6, and 8) in a [0°/90°n]s stacking sequence are tested using a split-Hopkinson pressure bar (SHPB) apparatus equipped with digital image correlation (DIC). The results depict the increase in the compressive strength as the strain rate increases from ~300 s⁻¹ to ~1200 s⁻¹. The ultra-high-speed camera captures the damage propagation in the specimens to further understand the failure mechanisms and dominating failure modes. The reported damage propagation provides insights over the interfacial properties (inter-and intralaminar interfaces) and the dynamic crack speed in fiber-reinforced composites. Post-mortem investigation of the deformed samples using scanning electron microscopy revealed features including fiber-matrix debonding, fiber breakage, fiber kinking, and loose fibers resulted due to the in-plane loading direction. Additionally, development of fracture plane within the 90° plies has been observed during the experiments showing the evidence of inter-fiber failure mode. This work aids towards in-depth understanding of the influence of the number of plies in a cross-ply composite laminate and validation cases for high-fidelity numerical models evaluating the dynamic mechanical and interfacial properties for aerospace, defense and automotive industries.</td>
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### 12 pm – 12:20 pm, May 24
**AFTP19:** Load bearing capacity and operational effectiveness of Single Shear Joints of CFRP Composite Laminate with Spread Tow Thin Piles  
**Tabrej Khan,** Prince Sultan University  
**Abstract:** Spread-tow thin-ply-based technology has resulted in the progress of optimized reinforced composite plies with ultra-low thicknesses. There is wide use of composite bolted joints in the aircraft industry for load-bearing structures and are regarded as the primary source of stress concentration. The purpose of this study is to look into the bearing strength and structural performance of single shear bolt joint configurations in composite laminates which are basically a combination of conventional thin-plies and thick-plies in some specific stacking sequence. The placement effect of thin-ply within the configured stack on bearing strength, as well as the potential damages, were investigated. Mechanical tests were used to understand the disfigurement mechanisms of the plies and their reciprocity, as well as to reflect on the single shear bolt joint properties and its load-bearing capacity. The results showed that changing the configuration of laminates by inserting the thin plies inside, improved the bearing strength by up to 19%.

### 1:40 pm – 2 pm, May 24
**AFTP20:** Developing a Platform for the Optimization and Quality Control Management of a Perfusion Cannula Fabrication Process  
**Anthony Demong,** University of Calgary  
**Abstract:** Cardiovascular disease is a leading cause of death, prevalent throughout the modern world. Fortunately, advances in cardiovascular medicine are being constantly developed, including the use of extracorporeal (i.e., out-of-body) circulation to temporarily bypass defective tissues during heart surgeries, transplants, and other critical medical procedures. Extracorporeal circulation involves diverting blood flow outside of the body using perfusion cannulae: biocompatible, coil-reinforced tubes designed for insertion into blood vessels to facilitate the transport of blood. Cannulae are produced using a dip-coating process that involves immersing a preheated mandrel into a liquid polymer bath. Heat then transfers from this mandrel to the surrounding polymer, resulting in the formation of a gel-like coating that, after additional heating at specific temperatures, fuses into a durable, rubberlike cannula tube. However, despite the critical role of perfusion cannulae in various surgical procedures, there is a gap in public knowledge detailing how to fabricate cannulae in a consistent, controlled manner. As surgeries that require perfusion cannulae become more frequent, there is a growing need for a more comprehensive understanding of cannula fabrication techniques beyond empirical design. In partnership with local Alberta company Ecmius Biomedical, this research seeks to enhance perfusion cannula fabrication processes through the development of a robotic dip-coating control system. Utilizing integrated sensors, imaging equipment, and computer-vision analysis techniques, this platform will provide a deeper understanding of the dip-coating polymer deposition process and the relative importance of its various process parameters. By shifting from traditional empirical methods to a more data-driven, analytical approach, this system will enable cannula manufacturers to achieve the level of precision and quality control essential for the manufacturing of medical devices.

### 2 pm – 2:20 pm, May 24
**AFTP21:** Fabrication of Durable and Inextensible Silicon Rubber Molds Tailored for high-Pressure Embossing of IR Transparent Materials  
**Abolfazl Vaheb,** University of Alberta  
**Abstract:** This study develops a manufacturing technique using fiberglass-reinforced silicone rubber molds for replicating structured polyethylene sheets, aimed at modifying thermal infrared (IR) properties. It addresses the challenge of molding thin layers without deforming under high pressure, a common issue with standard silicone rubbers. Our method, which contrasts with traditional soft lithography's particle reinforcement, utilizes thin woven fiberglass for mold strength, allowing for high-pressure molding while maintaining mold flexibility and ease of demolding. This approach is optimized for soft lithography, typically involving lower pressures and thermoset materials, rather than thermoplastics. Ensuring dimensional stability in thermoplastic sheets replication requires integrating fiber with silicone to avoid bubbles and prevent mold layer separation. Achieving thin, uniformly bonded fiberglass layers within the silicone is essential to prevent delamination at high pressures and temperatures (~1000 psi, >150 °C). Our study focused on creating precise, thin silicon layers crucial for bonding with microstructures, using TC-5030 and Sylgard 184 PDMS materials on a spin-coater. We achieved a 30μm minimum thickness with TC-5030, essential for fiberglass integration. By bonding two thin (~30μm), partially cured silicone layers and employing vacuum packing before curing, we ensured compactness and minimal distortion during high-pressure embossing, enabling precise placement of holes/structures near the fiberglass reinforcement.

### 2:20 pm – 2:40 pm, May 24
**AFTP22:** Curvy mechanical metamaterials for fracture resistance, energy absorption, and vibration isolation applications  
**Ramin Hamzehei,** University of Manitoba  
**Abstract:** This research shows the significant effect of curvy metamaterials on fracture toughness, energy absorption and vibration isolation. The conventional re-entrant unit cell is first reformulated by introducing local
curvy ligaments, leading to a decrease in structural stiffness. Different curvature of curvy unit cells leads to variability in structural stiffness. This provides an opportunity to consider different curvy unit cells corresponding to different engineering applications. The low-stiffness curvy unit cells, for example, can release stress concentrations in the notch areas, providing more ductility and fracture toughness under tensile loads. Besides, a combination of high and low stiffness unit cells can exhibit plateau region (zero stiffness) on force-displacement relation under compression. This zero-stiffness feature can considerably decrease the natural frequency of the system, resulting in isolating external excitations. Consequently, this study shows how curvy lattice structures can be used effectively in the enhancement of some mechanical features, including fracture toughness, and vibration isolation.

2:40 pm – 3 pm, May 23
AFTP23: Organogel Coatings to Shed off Mud/Ice/Slush Contaminants
Lin Zhitong, University of Alberta
Abstract: Outdoor surfaces in colder climates can often suffer from the undesired attachment of ice, mud, and slush especially when it snows. Often, forceful actions are needed to remove these foulants but can easily cause damage to the surfaces. Here, we propose one possible solution of using organogels as a top layer to shed off the foulants with simple stretching actions. Silicone-based organogels are designed with nanopores to hold oil lubricants inside which decreases the surface affinity to foulants. The high elasticity of the organogel coating enables stretchability, leading to the release of lubricants and subsequent removal of contaminants when stretched. The affinity among the organogel, lubricant and contaminants is carefully designed to minimize oil depletion. The shedding-off performance is evaluated using a setup in the lab which mimics the various winter conditions.

3:20 pm – 3:40 pm, May 24
AFTP24: An endeavor to develop a novel analysis approach for characterizing the time-dependent behavior of PE pipes
Furui Shi, University of Alberta
Abstract: Polyethylene (PE) provides significant advantages over other materials because of its good chemical resistance and appealing mechanical properties. For applications in water and gas transportation, the latest generation of PE pipes could have a lifetime more than 100 years. During such a long service life, complicated time-dependent deformation behavior of PE pipes is manifested, but its influence on mechanical performance is yet to be fully understood and characterized. We have recently developed a multiple-relaxation-recovery (RR) test to characterize the time-dependent mechanical performance of PE, and used the test to evaluate three grades of PE pipes. The test results were analyzed using a spring-dashpot model with three branches to represent quasi-static, long-term viscous, and short-term viscous stress responses, with the Eyring’s Law to govern the deformation of the dashpots. Although a computer algorithm has been developed to determine values for the model parameters in order to mimic closely the RR test results, the algorithm is not suitable for test results from PE pipes due to the lack of a plateau region in the stress-deformation curve to establish the trend of change of the model parameters that will be used to characterize the PE pipe performance. Therefore, we are currently searching for a new analytical approach to establish the trend of change. This presentation will firstly introduce the original algorithm and the results for three PE pipes, and then propose the idea for the new analytical approach. As an on-going investigation, the presentation will also update the progress in the development of the new algorithm and the improvement in the data analysis. It is envisaged that with the successful development of the new algorithm, mechanical performance of the three PE pipes could be fully characterized, which will be used to identify a direction for improvement of PE pipes so that their service capacity can be further increased.
**Abstract Appendix**

**10:20am - 10:40am, May 23**

**AMSE1: (Invited)** Design of Stable Nanocrystalline Multicomponent Alloys Towards Carbon Emission Reduction

**Ahmed Tiamiyu, University of Calgary**

**Abstract:** Energy-efficient/low-emission structures are vital for sustainable urban development, particularly in the fight against global climate change. Energy and transportation sectors prioritize sustainable development goals through the use of lightweight materials in structures. The current approach to lightweight often sacrifices the strength of the materials. This talk will focus on the next frontier in lightweighting technology that requires the development of nanocrystalline (NC) structure. This is because reducing grains to the nanoscale increases materials' strength and, in turn, reduces materials' thickness and weight requirements for structural components. While NC materials are attractive in principle, their extensive adoption has been hindered by the occurrence of significant growth of nano-crystals, even at room temperature, leading to a decrease in mechanical and functional properties while in use. A well-established strategy to address this thermal instability for binary alloys is by doping the host solvent with a solute that prefers to decorate the grain boundaries (GBs) rather than remain in the grain interior of the host—a process that offsets the excess energy at the GBs that drives coarsening. This talk will cover the newly discovered novel method (termed pseudo-binary thermodynamic approach) for stabilizing NC multicomponent alloys using high-entropy alloy (HEA) as the solvent. The thermodynamic stabilization approach guided by empirical and GB-segregation enthalpy considerations for binary-alloy systems will be discussed. Additionally, commercial adoption of NC materials to date is processing paradigms that are based on “bottom-up” growth processes, like electrodeposition methods. These techniques can develop materials with grain sizes below 100 nm but are limited in thickness, ~1-100 µm. This talk will also cover our current efforts to push beyond the thickness limitation to develop bulk stable NC-materials for lightweight structural applications.

**10:40am - 11:00am, May 23**

**AMSE2:** Solid Removal in the Warm Lime Softening Process of SAGD Water Treatment: Effects of Coagulant and Flocculant

**Siyu Li, University of Alberta**

**Abstract:** The treatment of produced water and its cyclic use play a critical role in steam-assisted gravity drainage (SAGD) operations for extracting bitumen from oil sands. The buildup of silica and hardness deposits results in scaling and blockages in pipes, equipment, and other surfaces, leading to decreased efficiency and higher maintenance expenses. The complex composition of SAGD produced water, along with a limited understanding of the fundamental molecular aspects and interactions involved in the warm lime softening (WLS) process and coagulation-flocculant treatment, has received considerable attention. In this work, we investigate the performance of solid removal and reduction of hardness using different coagulants and flocculants under simulated WLS processing conditions and reveal the interaction mechanisms underlying the coagulation-flocculation process using analytical tools such as focused beam reflectance measurement (FBRM) and surface force measurements. The results from this study indicate that the primary mechanism for the removal of silicon elements, the adsorption onto magnesium hydroxide precipitates. The addition of coagulants and flocculants aids in the formation of larger flocs, enhancing the sedimentation process and effectively removing a significant amount of particles. Moreover, there is a positive correlation between temperature elevation and silicon removal efficiency was observed, with optimal performance achieved at temperatures ranging from 70 to 85 °C. These findings align with real-world industrial practices. Our results provide useful insights into the fundamental understanding of the interfacial phenomena during the coagulation/flocculation process for removing silica and hardness in SAGD operations, with useful implications for the development of novel coagulants and flocculants with a wide range of applications in the oil and chemical industry.

**11:00am - 11:20am, May 23**

**AMSE3:** Tailoring Cu valence states in co-catalysts on ZnTe/ZnO photocathodes for syngas production

**Yi-Cheng Wang, University of Alberta**

**Abstract:** The mixture of CO and H2 is commonly known as syngas. Depending on the feedstocks and types of process such as the production of polyurethanes and dimethyl ether, etc., a specific ratio of CO and H2 is necessary. Nowadays, syngas is mainly produced from reforming or partial oxidation of fossil fuels, which is always energy intensive and accompanied with large amounts of CO2 emission, eventually triggering the greenhouse effect. In other words, the production of syngas with tuneable CO/H2 ratio with renewable energy and controlled pollution is expected. By and large, photoelectrochemical CO2 reduction reaction (PEC CO2RR) is believed one of the most promising strategies for not only utilizing solar energy but also achieving carbon-neutral sustainability. However, the poor selectivity and lack of suitable p-type semiconductors make the development of efficient photocathode driven syngas production systems very challenging. As a result, loading co-catalysts to accelerate the surface reaction kinetics and improve syngas selectivity is supposed to be an effective approach. In particular, Cu has...
Abstract Appendix

appropriate binding strength with the intermediates during CO2 reduction, thus exhibiting good potential in PEC CO2RR. However, the chemical state of the Cu surface is always difficult to control and identify, while the valence state usually has a great impact on the catalytic process. Therefore, the role of Cu valence state in PEC CO2RR has attracted more and more attention. Herein, a simple method of loading Cu2−xTe co-catalysts onto 1% S-doped ZnTe/ZnO by using different wavelength of light to control the chemical valence state of Cu between +1 to +2 has been proposed. With shorter deposition wavelength, the valence of Cu reduces, resulting in suppressed hydrogen evolution reaction (HER). As a result, Cu@S-ZnTe/ZnO shows a tuneable CO/H2 molar ratio in the range of 0.45 to 1.70, demonstrating the great potential of Cu@S-ZnTe/ZnO for practical PEC CO2RR application.

11:40am - 12:00pm, May 23
AMSE4: (Invited) Challenges and prospects for the application of AI tools for the design and optimization of green energy materials
Chandra Veer Singh, University of Toronto
Abstract: (Invited) Developing new energy materials technologies are the key to enable global energy transition to renewable energy. However, new materials development often takes many years. Artificial intelligence (AI) tools have emerged as new paradigm for materials development as they can reduce this materials discovery-deployment cycle by finding hidden patterns in material behavior and allow quick computational screening of promising material designs to guide experimentation. In this talk, we would describe the role of data sciences, particularly machine learning, coupled with atomistic simulations, to design and explore novel materials for sustainable energy applications. The following representative examples will be discussed: (a) design of champion materials for solar-driven CO2 reduction, thereby mimicking photosynthesis; (b) role of 2D materials in improving capacity and performance of lithium-ion and lithium-sulfur batteries; and (c) AI enabled design of high entropy alloy (HEA) catalysts for key energy conversion technologies key: CO2 reduction to useful chemical fuels, green ammonia production, and hydrogen evolution reaction. We will also discuss concurrent challenges and prospects. These works will also serve as an example of how we can combine data science with atomistic modeling and experimental testing to design next-generation materials to combat global warming.

12:00pm - 12:20pm, May 23
AMSE5: Mesoporous BiVO4 -based Photoelectrode in Water Splitting Photoreactor
Ali Tavazohi, University of Alberta
Abstract: In this study, heterostructure of SnO2/BiVO4/MoS2 has been introduced as potential photoanode for photovoltaic-electrochemical water splitting. In this configuration, tin oxide acts as a support layer and electron transport layer to the FTO and BiVO4/MoS2 have absorber layer role. Appropriate bandalignment between MoS2, BiVO4, and SnO2 caused desirable charge separation and O2 generation. To evaluate the phase and stability properties of photoelectrodes, XRD analysis was conducted prior and after PEC water splitting test to elucidate pure rutile tetragonal SnO2, monclinic BiVO4, and hexagonal MoS2 formation before contacting electrolyte as well as their stability after operation. Also, FESEM imaging has been carried out not only to identify the morphology and porosity of SnO2, BiVO4, and MoS2 but also to assess the morphological changes after 1 hour test operation. In the case of photovoltaic-electrochemical performance properties, gas chromatography and electrochemical characterization methods, including linear sweep voltammetry, cyclic voltammetry, chopped current-time, and amperometric (current-time), has been conducted, which implies great photocurrent and gas generation of SnO2/BiVO4/MoS2 rather than SnO2/BiVO4 photoanode.

12:20pm - 12:40pm, May 23
AMSE6: Nanoindentation studies of halide perovskites
Ruitian Chen, University of Toronto
Abstract: Halide perovskites stand out as promising photovoltaic materials in solar cell research, showcasing exceptional energy conversion efficiency. While significant strides have been made in understanding their optoelectronic properties, there remains a notable gap in the exploration of their mechanical behavior, an aspect crucial for comprehending material stability and robustness. In this study, we utilize the nanoindentation testing method, renowned for its efficacy in quantitatively obtaining various mechanical properties from very small volumes. Through this approach, we systematically delve into a series of single crystals of halide perovskites. The investigation, supplemented by additional characterizations, provides valuable insights into the trends of their mechanical behaviour. This work ensures a more comprehensive understanding of halide perovskites, contributing to the advancement of their practical applications.

02:40pm – 03:00pm, May 23
AMSE7: (Invited) Quantifying opportunities and challenges of disruptive processes for future production of zero-CO2 FeMn alloys
Sami Meddeb, Emeral Ideas
Abstract: (Invited) High-throughput primary production of FeMn alloys will remain vital to the industry for the next decades for meeting the demand for steels and non-ferrous alloys. The associated processes must shift towards sustainability, including the urgent need to cut their net CO2 emissions. Upgrading of existing plants is possible and necessary (e.g. use of biogenic carbon, carbon capture), but the development of disruptive processes holds great potential for best compromises between performance (productivity and quality) and sustainability. Direct H2-reduction is an attractive method for iron, however ferroalloys of less noble metals such as Mn, Si, and Cr require other approaches to fully reduce their oxides (e.g. high-throughput electrolysis, plasma). The aim of the study is to provide a comparative review of the possible processes for zero-CO2 production of FeMn alloys, allowing to quantify the key
Abstract: The lightweight nature of magnesium (Mg) and its alloys makes them particularly appealing for enhancing energy efficiency across diverse industrial sectors. Mg exhibits various deformation modes, including distinct dislocations and twins, yet the initiation of plasticity and their correlation to different modes and their association with various grain orientations remain poorly understood. This study delves into the incipient plasticity within nanoscale deformed regions within a Mg-2 wt.% Gd coarse-grained alloys through nanoindentation, focusing on 13 distinct grain orientations. Grain orientations were meticulously chosen covering a range of distinct indentation Schmid factors for target deformation modes. Within each grain, >100 indentations were performed to ensure reliable statistical results. The tendency of orientation-dependent plastic deformation aligns well with the predictions of Finite-Element simulations. The initial pop-in stress measured in the load-displacement curves, likely associated with the nucleation stage, agrees with the other theoretical stress values found in the literature. The current study seeks to establish correlations between the statistical characteristics of experimental pop-ins and the statistical nature of nucleation events.

03:00pm – 03:20pm, May 23
AMSE8: Mechanism on mechanical degradation and microstructure evolution of a Cr-Mo steel over long-term service
Zhe Lyu, University of Alberta
Abstract: The microstructure of both new and 40-year service-exposed 1Cr-0.5Mo steel was extracted through boat sampling techniques from pressure vessels were characterized in detail, through x-ray diffraction, field emission microscope, energy dispersive spectroscopy, electron backscatter diffraction, focused ion beam, and transmission electron microscopy. Mechanical testing of the samples from both conditions were also performed on sub-sized tensile samples. Compared with the new 1Cr-0.5Mo sample, the service-exposed samples were significantly embrittled, as characterized by almost twice the increase in yield strength and 23% loss of ductility. Thermodynamic and kinetic calculations were performed to understand the formation kinetics of the Mo2C carbide over long-term service at elevated temperatures. Quantitative correlations between mechanical properties and microstructure were also achieved through the development of statistical crystal plasticity models, which confirms that the nanoscale Mo2C carbides nucleated within the ferrite matrix over the long-term service results in a significant strengthening of the matrix. On the other hand, the coarser grain boundary Cr23C6 carbides, act as the damage accumulation sites and lead to degradation.

03:20pm - 03:40pm, May 23
AMSE9: Orientation-dependence of Incipient plasticity in Mg-Gd alloy by nanoindentation
Moein Imani Foumani, University of Manitoba
Abstract: The lightweight nature of magnesium (Mg) and its alloys makes them particularly appealing for enhancing energy efficiency across diverse industrial sectors. Mg exhibits various deformation modes, including distinct dislocations and twins, yet the initiation of plasticity and their correlation to different modes and their association with various grain orientations remain poorly understood. This study delves into the incipient plasticity within nanoscale deformed regions within a Mg-2 wt.% Gd coarse-grained alloys through nanoindentation, focusing on 13 distinct grain orientations. Grain orientations were meticulously chosen covering a range of distinct indentation Schmid factors for target deformation modes. Within each grain, >100 indentations were performed to ensure reliable statistical results. The tendency of orientation-dependent plastic deformation aligns well with the predictions of Finite-Element simulations. The initial pop-in stress measured in the load-displacement curves, likely associated with the nucleation stage, agrees with the other theoretical stress values found in the literature. The current study seeks to establish correlations between the statistical characteristics of experimental pop-ins and the statistical nature of nucleation events.

03:20pm - 03:40pm, May 23
AMSE10: (Invited) Synthesis and Evaluation of Nanostructured High-Entropy Alloy Films as Advanced Catalysts for Water Splitting
Daniela Arango, Natural Resources Canada
Abstract: Developing active, stable, and cost-effective electrocatalysts is essential for achieving efficient hydrogen production through water splitting. Nanostructured high-entropy alloys (HEAs) have gained considerable attention as electrocatalysts due to their abundant active sites, diverse elemental compositions, and tunable properties. This study investigates the synthesis and electrochemical activity of noble-metal-free HEA films. To accomplish this, Ni-Fe-Co-Mo-W(Cr) HEAs were electrodeposited on a carbon cloth and subjected to corrosion post-treatment to achieve a metal (oxy)hydroxide-rich surface. A comprehensive characterization of the obtained catalysts involved electrochemical techniques such as linear sweep voltammetry and chronocoulometry. Additionally, scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDX) and X-ray photoelectron spectroscopy (XPS) was employed to analyze the morphologies and compositions of the final coatings. Both the electrodeposition parameters and alloy composition demonstrated a significant impact on the performance of the final alloys. Moreover, the treated electrocatalysts exhibited enhanced hydrogen evolution reaction performance, and notable stability. These findings significantly enrich our understanding of HEA material engineering, providing insights into the development of sustainable and efficient electrocatalysts for hydrogen production through water splitting.
Abstract

AMS11: Atomic structure and thermal behavior of FeCoNbYB bulk metallic glass with high glass forming ability and excellent soft magnetic performance

Amir Hossein Taghvaei, Queen's University

Abstract: Fe-based bulk metallic glasses (BMGs) are state-of-the-art soft magnetic materials widely utilized in power electronics and electrical machines for efficient energy generation, transmission, and conversion. Their appeal lies in their low core losses, high saturation magnetization (Ms), and low coercivity (Hc). To further enhance their thermal stability and soft magnetic performance, a comprehensive investigation into the atomic structure and its evolution during annealing, along with the crystallization kinetics of Fe-based BMGs, is imperative. In this study, a FeCoNbYB BMG rod was fabricated through copper mold casting and its isochronal crystallization kinetics, structural relaxation, and the evolution of magnetic properties during annealing was studied. The as-cast FeCoNbYB BMG exhibited a high glass-forming ability (up to 4 mm diameter), a wide supercooled liquid region (SLR) of 98 K, extremely low Hc (1 A/m), and a moderate Ms of 92 Am2/kg. High-energy synchrotron X-ray diffraction (XRD) revealed an anomalous liquid-liquid phase transition (LLPS) in the SLR, accompanied by an increase in medium-range order (MRO), correlation length, and enhanced connectivity of solute-centered clusters. It was demonstrated that the LLPS is responsible for enhanced thermal stability, GFA and improving the magnetic behavior, such as increased Curie temperature (from 550 K to 580 K) and Ms (from 92 to 97 Am2/kg). Crystallization behavior indicated the formation of major (Fe,Co,Y)23B6 crystals and a small quantity of (Fe,Co)3B phase, with high activation energies of 530 kJ/mol and 804 kJ/mol for the first and second crystallization peaks, respectively. It was demonstrated that the Johnson-Mehl-Avrami-Kolmogorov (JMAK) approach is not applicable for describing crystallization kinetics, due to the complex and autocatalytic nature of crystallization in isochronal model and the Şesták-Berggren (SB) model providing more reliable results.

AMS12: Electrochemical CO2 fixation and conversion to green urea

Sourav Paul, Ramakrishna Mission Vidyamandira

Abstract: 150 million tons of urea is produced annually across the globe and forms the core of the fertilizer sector. Industrial production of urea involves application of high temperature and elevated pressure; it is not only a capital-intensive process but also environmentally hazardous one. So, looking into the future of carbon neutral society, we present an innovative solution to produce green urea at STP by electro catalysis. However, single step electrochemical green urea synthesis process is significantly hindered due to the absence of efficient and economically viable electro catalyst with multiple active sites for dual reduction of N2 and CO2 gases to produce urea. In this work, we showcase a wonder molecule from transition metal phthalocyanine family supported on MoS2. Herein, we report that cobalt phthalocyanine embedded on MoS2 matrix (CoPc–MoS2) as an efficient electro catalyst which exhibits excellent urea yield of 175.6 µg h-1 mg-1cat and FE of 15.12 % at ~0.7 V vs RHE by co-reduction of N2 and CO2. The dual metal center of Co and Mo in CoPc–MoS2 mediates the vital C–N bond formation by effective N2 activation by polarization, thereafter CO (produced from CO2RR) insertion followed by protonation to produce urea. The CoPc–MoS2 interfacial coupling interaction played an essential role in synergistic stimulation of the Mo-edge sites of MoS2 and the multiple active sites of CoPc (metal center, Pyrrolic and Pyridinic nitrogen) toward the urea synthesis, while concurrently protecting the exposed sites from competing HER.

AMS13: Acid–base chemistry and the economic implication of electrocatalytic carboxylate production in alkaline electrolytes

Mohammad Arshad Muzibur, University of Alberta

Abstract: Recent advancements in renewable energy technologies underscore the potential for sustainable chemical production via electrochemical systems. This study explores the techno-economic challenges associated with the electrocatalytic production of carboxylates in alkaline electrolytes, a process traditionally favored for its efficient kinetics and lower operational costs. However, the dissociation or deprotonation of organic acids in these high pH environments complicates downstream product separation and electrolyte recovery, significantly inflating capital and operational expenses. Our analysis specifically examines the glycerol oxidation to glycolic acid in alkaline conditions, revealing that over 60% of the production costs are attributed to the separation processes required to manage the resultant potassium salts. Our TEA results concluded that for production of 1 kg of Glycolic Acid, the entire process consumes 1.09 Kg of KOH, 0.96Kg of H 2 SO 4 for neutralization and generates an excess of 1.7 Kg K 2 SO 4 as a by-product. This essentially means that Glycolic Acid becomes the byproduct and K 2 SO 4 as the main product. The substantial economic burden imposed by these separation requirements highlights a critical oversight in current research focused predominantly on catalyst development without adequate consideration of subsequent separation challenges. The findings emphasize the need for a holistic approach in the development of electrochemical processes, suggesting that future research should also address the integration of efficient separation technologies. This could potentially include innovations in catalyst design that reduce the dependency on alkaline environments or alternative electrolytic systems that mitigate the formation of problematic byproducts.
Abstract Appendix

AMSE14: (Invited) Structural Design and Electrochemical Potassium Storage Properties of Metal Chalcogenides
Yuhan Wu, Shenyang University of Technology
Abstract: In next-generation electrochemical energy storage systems, potassium-ion batteries (PIBs) have been considered as a promising alternative to lithium-ion batteries by virtue of their suitable working potential, high safety, and cost competitiveness. Nonetheless, such an emerging energy storage technology is still unable to compare with lithium-ion batteries possessing extensive research and commercialization experience. One of the main constraints is the unsatisfactory electrochemical performance of PIB anodes. So far, a variety of materials have been explored to serve as candidates, such as carbon materials, metal oxides, alloying materials, organic materials, etc. Among them, metal chalcogenides are attractive due to their relatively high capacities, great redox reversibility, and easily controlled morphologies. Herein, we explored the electrochemical K+ storage possibility, behaviors, capabilities, and reaction mechanisms of some metal chalcogenides as PIB anode materials. Then, the electrochemical performance and stability were attempted to improve by various engineering strategies.

10:40am - 11:00am, May 24
AMSE16: Effect of T4 and T6 Heat Treatment on the Microstructure and Conductivity of the Aluminum Alloy A356
Kyle Lessoway, The University of British Columbia – Okanagan
Abstract: The aluminum alloy A356 is commonly used in transmission cases, engine heads, and some structural components in aerospace and automotive applications. It is known for its good strength, excellent castability, high corrosion resistance, and low density. This work investigated the behaviour of the cast A356 alloy throughout a T4 and T6 treatment process, including a thorough evaluation during the natural aging processes. The T4 and T6 treatment significantly increased the alloy’s mechanical properties and conductivity. The electrical conductivity increased with the refinement of the silicon eutectic phase and further with the precipitation of the Mg2Si phase with artificial aging. The increase in hardness was attributed to the precipitation of the Mg2Si and the refinement of the eutectic silicon phase, which also contributed to a 30% increase in tensile strength and 130% increase in ductility. The optimal samples were analyzed for high-temperature (25-275°C) electrical and thermal conductivity to evaluate the operating properties of the castings when used at elevated temperatures.

AMSE15: Chalcogenide nanoparticle sensitized TiO2 nanotube arrays for photocatalysis and photoelectrochemistry
Damini Vrushabendrakumar, University of Alberta
Abstract: We report on the improved photocatalytic and photoelectrochemical performance of TiO2 nanotube arrays (TNTAs) sensitizing to visible photons by decorating them with chalcogenide nanoparticles (NPs) made of CdSe, CdTe, PbSe, and PbTe. The TNTAs are synthesized using electrochemical anodization process. Two distinct methods are employed to form the chalcogenide nanoparticles on TNTAs: electrodeposition and successive ion layer adsorption and reaction (SILAR). The incorporation of specific chalcogenide nanoparticles into the TNTA structure is selective to the precursors employed, and their size can be controlled by adjusting precursor concentrations, electrochemical potential, and deposition duration. CdSe NP decorated TNTA heterostructures are comprehensively characterized for their structural and optical properties. Chalcogenide sensitization effectively broadens and intensifies light absorption. Photoluminescence (PL) analysis shows a pronounced blue shift in the emission peak compared to bulk chalcogenides indicating that a major portion of the decorated nanoparticles are in the quantum confinement regime and can be termed quantum dots. Evaluation of photoelectrocatalytic activity for water splitting demonstrates improved photocurrent density under visible light. The combined effect of TNTAs and chalcogenide nanoparticle decoration result in significant enhancements in overall water-splitting efficiency. This study offers valuable insights into the design of photoelectrodes for solar-driven water splitting and renewable energy applications. This research work extends the investigation of TiO2 nanotube arrays (TNTAs) sensitized with chalcogenide nanoparticles by evaluating their performance in photocatalytic CO2 reduction. The efficiency of the heterostructure in this process is assessed, offering insights into its broader applicability in sustainable energy technologies.

11:20am - 11:40am, May 24
AMSE17: (Invited) Self-extinguishing solid polymer electrolytes for solid-state lithium metal batteries
Yuhang Zhang, Shenyang University of Technology
Abstract: Solid-state lithium metal batteries are one of the most competitive candidates for next-generation energy storage devices due to their high safety and high energy density. The interface infiltration, flexibility, and plasticity of solid polymer electrolytes (SPEs) are better than those of inorganic solid electrolytes. Polyethylene oxide (PEO)-based SPEs have been widely studied among various polymer matrices. However, the migration of Li+ is inhibited due to the semi-crystalline state of PEO segments, leading to a low ionic conductivity at room temperature. Most modification strategies focus on improving the ionic conductivity but disregarding its inherent flammability that poses a substantial safety hazard. In this case, a self-extinguishing PEO-based SPE that combines excellent room-temperature electrochemical properties and high safety was explored via a solvent-free and high-efficient UV-derived free radical crosslinking reaction. The effect of different additives on electrochemical properties and cell performance was revealed, which may provide new perspectives for developing high-energy-density and high-safety lithium metal batteries at room temperature.
Abstract Appendix

11:40am – 12:00pm, May 24
AMSE18: Semi-metallic intrinsically decorated Ti-based oxide electrodes for electrochemical hydrogen generation

_Ula Suliman, University of Alberta_

Abstract: Green hydrogen, produced by electro-photocatalytic water splitting, is an energy dense and renewable energy source, and a promising candidate for a net-zero carbon fuel. Its cost limitations are exasperated by the low abundance of platinum group metals (PGMs), which represent the best performing water splitting catalysts. By effectively fabricating earth-abundant metals, and maximizing the utilization of PGMs, the cost bottleneck can be solved. Titanium dioxide is reported to be an excellent water splitting photocatalyst. However, electrocatalytic applications using titanium dioxide, a wide-band gap semiconductor, are hindered by its low conductivity and kinetic limitations. The nano-structuring of titanium dioxide, as well as the defect engineering using suitable reduction techniques, gives hope for its exhibition of semimetallic properties. The improved electronic properties make titanium dioxide a promising candidate as a highly efficient and stable metal oxide electrocatalyst support for single atom hydrogen evolution catalysts. The resultant electrode is a binder-free electrocatalyst that is directly coupled to the metal substrate. In this project, we report the reduction of self-assembled titania nanotubes. We investigate the intrinsic decoration of the nanotubes using copper-containing titanium alloy substrates followed by a high temperature treatment in Ar/H2. The titania-based electrodes were evaluated in electrochemical hydrogen evolution conditions, where they showed an improved performance in comparison to pristine titania.

12:00pm – 12:20pm, May 24
AMSE19: Importance of co-catalyst and surface adsorbate structure in CO2 photoreduction on TiO2 nanotube arrays

_Navneet Kumar, University of Alberta_

Abstract: Nanostructured TiO2 is a well-established photocatalyst for the sunlight-driven transformation of CO2 into value-added products. The anatase phase TiO2 nanotube array (TNTA) architecture is one of the best performing CO2 photoreduction catalysts (> 300 μmol/g/hr of products) due to high surface area, amphoteric surface with both Lewis acidic and basic sites, a nanotube wall-thickness comparable to the carrier diffusion length and a wide bandgap (~3.2 eV) providing enough thermodynamic driving force for the CO2 reduction reaction. What is particularly remarkable is that the same TiO2 nanotubes decorated with various co-catalysts generated disparate products such as light hydrocarbons (methylene, ethane and ethylene), formaldehyde and CO in the vapor phase photoreduction of CO2. For instance, 1-D photonic crystal TNTAs decorated with plasmonic Au nanoparticles reduced CO2 to methane under UV-rich sunlight and to formaldehyde using UV-filtered sunlight. CuPt decorated TNTAs transformed CO2 into light hydrocarbons with dominant methane while an ethane-dominant light hydrocarbon mixture was formed by TNTAs decorated with large AgCu nanoparticles. Sr-doped TNTAs photo-reduced CO2 to CO. Likewise, TiO2 nanotubes formed anodically in various electrolytes such as water, formamide (FA) and ethylene glycol (EG), exhibit different surface adsorbate structures which in turn influence the nature of the products formed and the product distribution. The surface adsorbate structure in TNTAs grown in EG consists of physisorbed linear CO2 molecules, and monodentate carbonate and bidentate bicarbonate species formed through chemisorption while the surface of TNTAs grown in FA also contain physisorbed and chemisorbed CO indicating direct transformation of adsorbed CO2 to CO in the dark.

01:40pm - 02:00pm, May 24
AMSE20: Data-Driven Design of Multifunctional Ceramic Components for Hydrogen Energy Applications

_Kasra Rezasefat, University of Alberta_

Abstract: Ceramic materials play a crucial role in the energy sector, offering unparalleled advantages in terms of durability, heat resistance, and chemical stability, which are necessary for the development and optimization of energy technologies. Particularly in the context of hydrogen energy, a key component of sustainable energy systems, the application of ceramics is expanding due to their potential to meet the high-performance requirements of hydrogen production, storage, and utilization systems. As the demand for advanced multifunctional materials capable of withstanding the harsh conditions associated with hydrogen applications grows, the need to design ceramic components with tailored properties has never been more pressing. This study focuses on employing data-driven approaches for the design of multifunctional ceramic parts tailored for hydrogen production applications. By leveraging additive manufacturing techniques alongside computational modeling and machine learning algorithms, our research seeks to create a framework for the development of ceramic components that fulfill the requirements of hydrogen technologies. We investigate the influence of processing parameters on the microstructure and functional properties of ceramics under operational conditions specific to hydrogen applications. The experimental effort includes characterization of ceramics to evaluate their mechanical properties, thermal resistance, and compatibility with hydrogen environments, employing techniques like SEM, X-ray computed tomography. The initiative of this work is expected to set new benchmarks for the integration of materials science, engineering, and data analytics, facilitating the development of advanced functional materials for the energy sector. This research serves to the immediate needs of the hydrogen industry and exemplifies the potential for innovative material solutions in energy applications, promoting sustainability and efficiency in the Canadian energy landscape.

02:00pm - 02:20pm, May 24
AMSE21: Innovative Ni-Fe Whiskers for Highly Efficient Oxygen Evolution in Alkaline Media

_Mohsen Fakourihassanabadi, University of Alberta_
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| **Abstract**: The development of efficient electrocatalysts is crucial for advancing energy conversion and storage technologies, particularly in the context of the oxygen evolution reaction (OER). This study focuses on mitigating OER overpotential, especially at high current densities, by employing high-activity catalysts coated on a 3D skeleton electrode with optimized pore design and a large specific surface area. Previously, we introduced a novel 3D structure of Ni (Ni-whiskers) characterized by optimized pore design and exceptional mechanical stability. This structure is achieved through the directional solidification of a Ni-Al eutectic alloy followed by leaching. Expanding upon this, we explore a promising catalyst synthesis method on Ni-whiskers by incorporating dopant elements into the structure. Here, we demonstrate the doping of Fe into Ni-whiskers using cyclic voltammetry and fine-tuning the Fe content within the structure. Our findings indicate that Ni-Fe whiskers exhibit significantly reduced OER overpotential in 1 M KOH electrolyte, with approximately 200 mV at 10 mA/cm² and, 300 mV for achieving a current density of 500 mA/cm². This work highlights the potential of Ni-Fe whiskers as efficient electrocatalysts for OER applications.

**02:20pm - 02:40pm, May 24**
**AMSE22**: Nanoengineered Zn-modified Nickel Sulfide (NiS) as a Bifunctional Electro catalyst for Overall Water Splitting

**Chandra Prakash, University of Alberta**

**Abstract**: Electrochemical water splitting is an essential electrocatalytic process for tackling the global issues of renewable energy sustainability and carbon management in the quest for a robust and sustainable future. Designing the nanoengineered and cost-effective electrocatalyst is pivotal requirement to boost the hydrogen production using electrochemical water splitting. This work will show the impact of the doping concentration of the Zinc (Zn) in the self-supported NiS on the Nickel foam (NF). The electrocatalyst (Zn-NiS-3) shows the better hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Zn-NiS-3 delivered the overpotential of 320 mV for OER and 208 mV for HER for current density 50 mA/cm² and 10 mA/cm² respectively. The Zn-NiS-3@NF shows the Tafel slope value 113 mV/dec and 36 mV/dec for OER and HER. The overall cell potential of the device is 1.71 V when Zn-NiS-3@NF used as anode and cathode. The enhance and superior performance of the Zn-NiS-3@NF is because of the high electrochemical surface area, low electrolyte/electrocatalytic charge transfer resistance, nano regime morphology, and tuning of the electronic property with doping of Zn in NiS@NF. Our aim is to improve the electrochemical performance of NiS by doping Zn on Carbon Cloth (CC), which is non-reactive to sulphur source in comparison to Nickel foam. This can provide both qualitative and quantitative impact of the Zn doping in NiS@NF or in NiS@CC.

**02:40pm - 03:00pm, May 24**
**AMSE23**: Novel Polyether Block Amide Polymers for Membrane-Assisted Decarbonization

**Arash Mollahosseini, Nanotechnology Research Centre, National Research Council Canada**

**Abstract**: Human daily life along side survival of many industries is intertwined with consumption of fossil fuels. Carbon emissions and other greenhouse gases from these activities take part in global warming and climate change. To mitigate climate change and manage the possible catastrophes, Albertan Government has focused on net-zero plan to be achieved by 2050. Affordable and scalable carbon capture technologies play a significant role in net-zero policies. One of the candidates to pursue the goal is membrane separation technology, which is an economical remedy with low environmental footprint for decarbonization. In last few years, poly ether block amide (PEBAX membranes have been extensively used due to their dipole-quadrupole interactions. However, standalone PEBAX membranes are not favorable due to limited mechanical stability and semi-crystalline structure. In this study we introduce a novel crosslinked PEBAX®@1657 membrane for carbon capture (or separation). And its crosslinked structure was assessed computationally through a simplified molecular dynamics simulation to understand the molecular interaction elements of polymer-CO₂. Single gas performance test reflected a CO₂ permeability of 18,000 Barrer with a CO₂/N₂ selectivity of 30. Computational simulations reflected an absorptive interaction energy of 335.36 kcal/mol for crosslinked pebax-CO₂, 68 Kcal/mol higher than pebax-CO₂. Higher share of electrostatic interactions reveals higher affinity of CO₂ molecules toward crosslinked PEBAX®@1657 chains. Based on this study, we developed low pressure modified membrane product for flue gas decarbonization. The findings of this research could benefit Alberta through facile and easy formulation change for role-to-role production lines’ feed to mass produce decarbonization membrane modules.

**03:20pm - 03:40pm, May 24**
**AMSE24**: Titanate photocatalyst/polyurethane foam composite for facile biohydrogen production via photo fermentation from corn stover

**Alemu getu Menegeste, Myongji University**

**Abstract**: Because of its short gas production cycle, environmental friendliness, and ability to use abundant and renewable biomass as a raw material, biohydrogen production via catalyst-assisted photo-fermentation is an appealing strategy. However, powder or particle-based photocatalysts are soluble in water, the recycling process is time-consuming, inefficient, and environmentally hazardous. To address these problems, we proposed immobilizing titanate photocatalysts (MgTiO₃) onto polyurethane foam (PUF). Using HAU-M1 bacterium and corn stover as a substrate, the developed MgTiO₃@PUF composite demonstrated excellent H₂ production performance, with a maximum yield of 563 mL per gram of sponge and a very high energy conversion efficiency of 36%. Furthermore, with a negligible decrease in H₂ production efficiency, the MgTiO₃@PUF photocatalyst can be successfully regenerated and reused for five cycles via simple squeezing. Unlike filtration membranes, the developed
Abstract Appendix

A foam-based catalyst has 3D interconnected large pores, resulting in negligible mass transfer resistance. Furthermore, the bulk structure of the foam makes the photocatalyst-foam composite easy to use and recycle without the use of a magnet or other energy inputs. Because of its exceptionally high H2 production efficiency, convenient operation, remarkable recyclability, and ease of separation, the obtained MgTiO3@PUF has enormous potential for H2 production via photo-fermentation in real-world applications.
**Abstract Appendix**

**Symposium:** Advances in Rechargeable Metal Batteries (ARMB)  
Friday, May 24, 2024  
Room: ECERF W2-090/110  
Chair: Zhixiao Xu

**10:00am - 10:20am, May 24**  
**ARMB1: (Invited) Impact of Pressure Distribution and Magnitude on the Performance of Lithium Metal Anodes**  
Matthew Li, Argonne National Laboratory  
**Abstract:** Li metal anodes play a pivotal role in battery technology by significantly enhancing the energy density of Li-based batteries. While the influence of pressure on the performance of Li-metal anodes is widely recognized, the specific impact of pressure values and distribution on performance remains ambiguous. Additionally, understanding the composition of the solid-electrolyte interphase formed under different pressure conditions is crucial for practical applications of lithium metal anodes. This study explores the effects of various pressure distributions achieved through differently shaped and oriented mechanical springs in coin cells, resulting in diverse contact points. Utilizing pressure-sensitive films, the pressure was spatially mapped and correlated with performance metrics. Surprisingly, we revealed that higher average pressure does not consistently improve performance. In instances where high pressure is coupled with uneven pressure distribution, performance deteriorates, likely due to a current focusing effect, leading to unstable cycling. This emphasizes the significance of managing the balance between average pressure and pressure uniformity for optimal performance.

**10:20am - 10:40am, May 24**  
**ARMB2: Viscoplasticity-Driven Suppression of Lithium Dendrite Penetration in Sulfide Electrolytes**  
Changmin Shi, Brown University  
**Abstract:** All-solid-state batteries (ASSBs) show a high practical potential to achieve safe battery design with high energy densities when using Li metal as an anode. Sulfide electrolytes due to their high ionic conductivity (0.1 mS/cm to >10 mS/cm) are among the most promising candidates. However, Li dendrite growth results in shorting at critical current densities (CCD) that are well below values that are needed for practical applications. Extensive efforts have been devoted to increasing the interfacial stability with methods that emphasize chemical and electrochemical modifications. However, methodologies that increase the CCD in sulfide electrolytes based on mechanics have not been reported. Herein we report a viscoplasticity based approach to increase the CCD of sulfide electrolytes. Previous studies have demonstrated that some sulfide SEs deform in a viscous manner. Considerations of this effect offer a new perspective on how to suppress Li dendrite growth. To investigate the viscoplastic properties of sulfide electrolytes, Li6PS6Cl was selected as an important candidate due to its high ionic conductivity and high stability against Li metal compared with other sulfide electrolytes. Viscoplasticity in this material was investigated and characterized by integrating nanoindentation experiments and finite element simulations, and improved CCD was observed by employing cycling conditions that take advantage of this inelastic deformation. Such improvement is attributed to the interaction between the specially designed charging-discharging cycles and the viscous deformation of the electrolyte. We have also performed finite element simulations to further validate our argument. This type of approach can provide major improvements in the performance of ASSBs and can also be combined with chemical/electrochemical methods to further enhance cell performance using sulfide electrolytes.

**10:40am - 11:00am, May 24**  
**ARMB3: 3D X-ray Computed Tomography Study of Si-C Composite Anodes in Li-Ion Batteries**  
Moin Abid, McMaster University  
**Abstract:** Silicon-based composite electrodes for lithium-ion batteries are garnering considerable attention due to their ability to serve as high-capacity substitutes for the traditional graphitic carbon anodes commonly utilized. However, their application is hindered by issues such as debonding and fracturing of Si particles, which are consequences of volumetric expansion experienced by the lithium host particles during the anode's lithiation. To investigate this, we employed X-ray computed tomography to track the changes in the internal microstructure of a Si-C anode at various stages: before lithiation, after the initial half-cycle of lithiation, following the formation cycle, and at the end of the lithium-ion cell's cycle life. In the lithiation phase of Si-C composite anode, initial cracking manifested on the outer surfaces of Si particles and advanced internally, signifying the material's mechanical stress response to volumetric expansion, a critical factor in understanding the dynamics of anode degradation. Simultaneously, the progression of lithiation is marked by diminished X-ray attenuation, denoting phase transitions within Si particles from crystalline to amorphous. Overall, this study shows the usefulness of X-ray computed tomography to study structure evolution in Li-Ion battery materials.

**11:20am - 11:40am, May 24**  
**ARMB4: (Invited) Beyond Lithium: Navigating the Landscape of Sodium-Ion Batteries with a Spotlight on Nanode's Breakthroughs**  
Jiankuan Li, Nanode Battery Technologies  
**Abstract:** The rapid growth of energy storage applications and technologies have been catalyzed by the pursuit of carbon neutrality. Lithium-ion batteries (LIBs) are projected to experience a significant surge in the upcoming decade, estimated to reach a demand of...
Abstract:

Sixu Deng, Concordia University

01:40pm - 02:00pm, May 24

ARMB7: (Invited) Development of High-Performance Inorganic Solid-State Battery Cathodes
Silk Deng, Concordia University

Abstract: Electric vehicles (EVs), representing the future of transportation, are predicted to be one of the ultimate solutions to eliminate greenhouse gas emissions. Li-ion batteries (LIBs), as the most promising sustainable energy devices, are critical for the development of EVs because of their higher operating voltages compared to other energy storage technologies. However, the development of conventional LIBs touched the ceiling because of three main challenges. (1) The use of flammable and toxic liquid electrolytes brings high safety risks. (2) The limited energy density of LIBs cannot satisfy the requirement for long-range EVs. (3) The increasing market demand for LIBs will cause resource shortages and a rise in cost. Accordingly, all-solid-state Li-ion batteries (ASSLIBs) have recently emerged as promising alternative batteries for next-generation EVs because of their ability to overcome the drawbacks of conventional LIBs. Among the developed solid-state electrolytes (SSEs), inorganic catalyst. As well, oxygen concentration cells that develop in open-to-air designs can corrode the inactive portion of the Zn electrode and lead to premature cell failure. Our research into viable mitigation strategies will be presented to help other Zn-air battery researchers in avoiding similar cell design pitfalls.

12:00pm - 12:20pm, May 24

ARMB6: Quantum Mechanical Investigation of Polyppyrole-MXene Nanocomposite as an Electrode Material for Magnesium-Ion Batteries
Anthony Ezika, Tshwane University of Technology Pretoria South Africa

Abstract: The current challenge in energy storage technologies lies in identifying efficient electrode materials for Magnesium-ion (Mg-ion) batteries, motivating the exploration of the energy storage capabilities of Polyppyrole-MXene nanocomposites as a potential solution to enhance battery performance. Hence, in this paper, quantum mechanical simulations are employed to examine the capability of energy storage of Polyppyrole-MXene filled nanocomposite. The electronic structures, adsorption energies, and adsorption site of Mg@PPy/MXene nanocomposite were investigated. The results reveal that Mg-ions on MXene/PPy nanocomposite have a very high adsorption energy of -0.84 eV. The distance of Mg-ion adsorption from the MXene’s surface at the bridge site is 2.75 Å. Its distance from the PPy, however, is considerably farther at 2.83 Å. The electron difference study, using the charge transfer analysis reveals that the dominating adsorption mechanism for the Mg-ion in the system is physisorption. The electrode’s propensity to transport electrons during the electrochemical reaction is shown by the projected density of state (PDOS) and its energy bandgap is 0.05. Consequently, the MXene/PPy nanocomposite might be used as an Mg-ion electrode in battery applications.

11:40am - 12:00pm, May 24

ARMBS: Challenges in Zn-Air Battery Cell Design
Matthew Labbe, University of Alberta

Abstract: As the push for more electric vehicles and more renewable energy sources increases, so too does the demand for energy storage. Electrochemical batteries are a well-developed energy storage technology that have reliably powered major advances in science. However, the ever-present Li-ion battery comes with several major drawbacks, including limited material resources and poor safety performance. As an alternative to Li-ion batteries, Zn-air batteries are attractive due to their lower cost, more abundant raw materials, and superior safety. Yet, Zn-air battery technology has not been as rigorously studied as its Li-ion counterpart. Important topics in Zn-air battery research include air electrode catalysis, Zn electrode reversibility, and electrolyte engineering. However, mechanical cell design is rarely discussed, despite the fact that it impacts the laboratory-scale performance and that there is no standard cell design among Zn-air battery researchers. Our research has found overlooked flaws in simple cell designs that can lead to erroneous conclusions regarding performance and failure. In particular, the material choice and placement of the current collector can inadvertently contribute to a modified catalysis mechanism. This can lead to undervaluing or overvaluing the efficacy of a potential...
sulfide and halide SSEs show great potential because of their excellent performance. For example, sulfide-based SSEs demonstrate high room-temperature Li⁺ conductivities (10⁻² to 10⁻³ S cm⁻¹), which have even surpassed those of conventional liquid electrolytes. Halide-based SSEs with a high electrochemical stable window realize along with a stable cathode interface. However, inorganic sulfide and halide ASSLIBs still face some key challenges hindering their application in EVs. In this talk, I will first introduce our studies on the cathode interfaces in sulfide ASSLIBs. After that, I will introduce our research on fast-charging and low-temperature halide-based ASSLIBs. Finally, I will introduce our findings on understanding the mechanism of inorganic ASSLIBs via synchrotron characterization.

02:00pm - 02:20pm, May 24
ARMB8: Organic-Pigment-Mediated Sulfide Electrolyte Redox for All-Solid-State Lithium–Organic Batteries with High Areal Capacity
Qihang Yu, Concordia University
Abstract: Organic electrode materials (OEMs) as one type of promising alternative for current transition metal oxides are dedicated to fabricating more sustainable lithium-ion batteries in the future. However, the high solubility of OEMs in the conventional liquid-based electrolyte severely restricted its development. As one of the several methods, using inorganic solid-state electrolytes fundamentally prevents the dissolution problem. Herein, we demonstrate that one typical organic material 2,2'-Bis(2,3-dihydro-3-oxoindolyliden) (Indigo) with argyrodite sulfide-based SSEs (Li6PSS5Cl) in All-solid-state batteries (ASSBs). With optimized carbon additives, Indigo-based ASSBs exhibit a high capacity of 535 mAh g⁻¹, a remarkable energy density of 1123 Wh kg⁻¹, and outstanding capacity retention of 86% at a high current density of 2C at room temperature. Moreover, these ASSBs with high active material loading (over 10 mg cm⁻²) are also constructed and showed a high areal capacity of about 3.75 mAh cm⁻² and excellent cycling performance (98%@100 cycles, 50 mA g⁻¹). Finally, to further investigate the electrochemical performance of Indigo-based ASSBs, the batteries are tested at a low temperature. The specific capacity is 250 mA g⁻¹ and no obvious loss of capacity during 100 cycles at 0.2C. These excellent electrochemical performances are attributed to the coordinated action of organic materials, electrolytes, and conductive carbon additives. Therefore, we believe this work not only demonstrates the good electrochemical performance of all-solid-state lithium-organic batteries at room temperature and low temperature but also reveals the potential of organic materials for future development in all-solid-state batteries.

02:20pm - 02:40pm, May 24
ARMB9: Self-healing and Polar Synergistic Multi-Functional Coating of Sulfur Cathodes for High-Performance Li-S Batteries
Zhao Yang, Concordia University
Abstract: The development of lithium-sulfur (Li-S) batteries is plagued by serious polysulfide shuttling, sluggish redox reaction kinetics, and low sulfur utilization. In this work, a multifunctional polymer designed as a sulfur/carbon coating layer with self-healability and polar groups is designed and prepared for Li-S batteries to achieve improved electrochemical performance. The dynamic poly(hindered urea) (PHU) polymer coating layer uniformly covered on the surface of the sulfur/carbon (S/C) composites acts as a physical barrier for the dissolution of lithium polysulfide (LiPSs) from the cathode to the lithium metal anode, which accumulates LiPSs on the cathode side and protects the lithium anode from corrosion. In addition, the dynamical and reversible self-healing hindered urea bonds (HUBs) endow the PHU coating layer with the ability to maintain structural integrity and stability even after numerous volume expansions and shrinkages of the S/C electrodes. More importantly, the polar groups carried by the PHU polymer exerted a strong adsorption effect on LiPSs, thus further hindering the shuttling of LiPSs. Consequently, the Li-S batteries using PHU coating layer exhibit impressive cycle stability (maintaining 82.8% capacity retention after 150 cycles at 0.5 C), and outstanding rate performance (capacity retention of 623.9 mAh g⁻¹ at 2 C). Furthermore, even under a high sulfur loading of 8.47 mg cm⁻², a high areal-specific capacity of 6.4 mAh cm⁻² is still delivered.

02:40pm - 03:00pm, May 24
ARMB10: Blocking Li Metal Dendrites with Piezoelectric Solid Polymer Electrolytes Through Coupled Piezoelectricity, Mechanics, and Electrochemistry Effects
Changmin Shi, Brown University
Abstract: Solid electrolytes (SEs) are very promising candidates to enable a safe battery design. However, “needle-shape” Li filament (Li dendrite) which can penetrate SE layer to cause battery electrically shorting, will be generated on the Li metal surface during battery charge process. This phenomenon typically occurs in existing SEs at a current density less than 1 mA/cm² at room temperature. The relatively low critical current density (CCD) severely limits fast-charge capability and the lifespan of solid-state batteries. Therefore, to promote the development of SEs in practical applications, it is urgent to improve the CCD of SEs. Herein we have introduced a novel piezoelectric solid polymer interlayer between SE and Li metal to serves as a robust barrier, effectively preventing Li dendrites penetration from the Li metal anode into the SE layer. To exemplify this approach, we utilized a cubic-structural Li7La3Zr2O12 as a representative SE material. Our innovation has resulted in a remarkable increase in the CCD of LLZO to the extent that our cells ceased operation due to reaching the upper voltage limit of the battery tester, rather than encountering electrical shorting issues. The excellent achieved performance is due to a coupled piezoelectricity, mechanics, and electrochemistry effects.
Abstract: The use of fossil fuels is one of the major causes of climate change and the transition from fossil fuels to renewable energies, such as wind and solar, is considered a promising strategy to tackle this problem. However, the supply of these renewable energies heavily depends on the weather conditions. To maintain a stable supply, the renewable energies can be electrochemically stored in batteries. Lithium-ion batteries (LIBs) have been utilized in portable electronic devices and electric vehicles, but their high cost limits their use in grid storage. In comparison, zinc-ion batteries (ZIBs) utilize zinc metal, which is roughly 5 times more abundant than lithium. ZIBs are also safer than LIBs because aqueous electrolytes can be used in ZIBs, whereas commercial LIBs use organic electrolytes that are flammable. However, at the zinc electrode, ZIBs suffer from dendrite formation, hydrogen evolution, zinc corrosion and by-production formation, which severely restrict the practical application of ZIBs. The electrolyte is a crucial component in ZIBs because it transfers charge carriers between the cathode and anode. The goal of this study is to use modified electrolytes with functional additives to mitigate ZIB issues and improve their performance. Potential functional additives are brighteners that have been used in zinc electroplating industries and additives that have high affinity with zinc. These additives can adsorb on the surface of zinc and guide uniform zinc deposition. Various characterization techniques, such as electrochemical testing, electron microscopy and X-ray diffraction, are used to investigate battery performance and explore the working mechanisms of the additives. Preliminary results indicate that the addition of functional additives can extend the lifetime of ZIBs, both in zinc-copper asymmetric and zinc-zinc symmetric cells.

Abstract: High performance CuHCF//Zn battery enabled by inner Helmholtz layer regulating co-solvent strategy

Abstract: Prussian Blue Analogues (PBAs) stands out as one of the most promising cathode materials, boasting significant advantages such as high working voltages, rapid reaction kinetics, decent battery lifespan, and low cost. Leveraging the benefits of PBAs cathodes in Aqueous-Zinc Ion Batteries (A-ZIBs) unleashes the full potential of the A-ZIB. For instance, PBAs cathodes uniquely exhibit working voltages at 1.7 ~ 1.8V, which is 50% higher than the common working voltage of around 1.2V in the A-ZIBs family, resulting in a more competitive energy density. Within PBAs, Copper Hexacyanoferrate (CuHCF) demonstrates reliable electrochemical stability, conductivity, and abundant resources. However, challenges arise from issues related to the formation of Zn(OTf)2·nH2O (ZOTFH) and the dissolution of Cu2+ ions driven by free water molecules at the inner Helmholtz layer, negatively impacting the performance of the CuHCF//Zn full battery. To address these challenges, a design employing a Methyl Acetate (MA) co-solvent with Zinc Triflate Zn(OTf)2 salt electrolyte is implemented. The MA co-solvent (75% vol.) successfully forms a solvation structure of [MA-OTf--H2O] or directly coordinates with water molecules, thereby inhibiting side reactions and preventing Cu2+ ion dissolution. This co-solvent electrolyte system enables the CuHCF//Zn A-ZIB to self-optimize its structure during cycling, maintaining 100% capacity retention for 2500 cycles over 3024 hours under the conditions of 1.33C, with an energy density of 108 Wh/g. Moreover, owing to the low viscosity and freezing point of MA, the CuHCF//Zn A-ZIB can operate at an extremely low temperature of -50°C, preserving half of its capacity in long cycle tests under ambient conditions.

Abstract: The interest in rechargeable zinc-ion batteries (ZIBs), as an energy storage replacement for lithium-ion batteries (LIBs), has increased in recent years. The advantage of zinc comes from its lower cost and better stability in aqueous systems. A ZIB is typically composed of two electrodes, a separator, and a liquid electrolyte solution. However, traditional separators made from fiberglass are vulnerable towards zinc dendrite formation and other side reactions that hinder battery cycling, causing cell failure. An alternative option to conventional separators is hydrogel or polymer electrolytes (PEs), which can serve as both the electrolyte and separator in ZIBs. Several polymers have been investigated for this purpose with the goal of improving cycling life and efficiency. In this work, polyacrylamide (PAM) is studied and is cast directly on the metallic zinc electrode. This fabrication process provides the ability to control the area and thickness of the separator/electrolyte layer.

Abstract: Surface electroactive sites of Tungstated Zirconia Catalysts for Vanadium Redox Flow Batteries

Abstract: Surface electroactive sites for tungstated zirconia (WZ) have been prepared using tungstate immobilized UiO-66 as precursors through a double-solvent impregnation method under mild calcination temperature. With moderate W (22%) contents, the as-synthesized WZ-22-650 catalyst possesses a high density of surface electroactive sites, and proper heat treatment leads to the binding of the oligomeric tungsten clusters to stabilized tetragonal ZrO2. The resultant WZ exhibits improved catalytic performance towards the VO2+/VO2+ redox couples among all the tested samples. In particular, the large surface area, mesoporous structure, and formation of new W–O–Zr bonds, all confirm that the WOx are anchored firmly to ZrO2, which can provide more surface electroactive sites to improve the electrochemical performance of VRFBs.
Charge-discharge tests further demonstrate that the superior voltage efficiency (VE) and energy efficiency (EE) of the VRFB using the WZ-22-650 catalyst are 87.76% and 83.94% at a current density of 80 mA cm$^{-2}$, which are 13.42% VE and 10.88% EE better than heat treated graphite felt (HGF), respectively. Even when the current density is increased to 160 mA cm$^{-2}$, the VE and the EE of VRFB using the WZ-22-650 catalyst still have 76.76% and 74.86%, respectively. The facile method endows the WZ catalysts with superior catalytic activities and excellent cyclability, thus opening a new avenue for preparing metal oxide-based catalysts.
10:20am - 11:00am, May 23
CPCE1: (Invited) Case Studies on Reducing CRM Dependency in Canadian Industries
Patrick Flood, InnoTech Alberta
Abstract: This presentation will examine the significance of Critical Raw Materials (CRMs) in Canadian industries, particularly mining, energy, and manufacturing. The rising use of critical minerals has prompted ongoing global efforts by Canada, the EU, the US, and others to identify and prioritize CRMs. These initiatives inform strategic planning to ensure sustainable access to CRMs and identify those crucial for various industries. Canada currently lists 31 CRMs, vital for strategic sectors and transitioning to a greener economy. This presentation will discuss three case studies illustrating the significance of CRMs that are extensively used within Canadian industries. The first case study examines the role of cobalt, nickel, and tungsten in wear-resistant materials used for mining and manufacturing equipment and will discuss potential alternatives and replacement materials. The challenge in this area is to maintain a similar level of performance in the intended application. The second case study investigates fluor spar and helium for welding applications. There is a current need to explore alternative welding processes, filler metal compositions, and gas mixtures to decrease the reliance on these CRMs without compromising welding quality. In the third case study, deliberate strategies to reduce the dependency on chromium for stainless steels in corrosive environments will be explored, particularly fabrication alternatives including materials selection, corrosion resistant coatings, and protective weld overlays. These case studies highlight the critical role of materials engineers in innovating to reduce CRM dependency. Opportunities for identifying material substitutions, process changes and optimizations, and recycling initiatives will continue to support sustainability efforts. By embracing sustainable materials design and resource management practices within a more circular economy, materials engineers will meaningfully contribute towards protection of our CRM assets.

11:00am - 11:20am, May 23
CPCE2: Magnesium Doping for Enhanced Stability of Lithium Manganese Oxide Ion-sieves for Lithium Recovery from Flowback and Produced Water
Fangshuai Wu, University of Alberta
Abstract: The global energy transition has led to a rapid increase in the demand for lithium, particularly in the use of batteries for electric vehicles and large-scale grid energy storage. To meet future requirements, the development of new lithium resources has become a necessity. Flowback and produced water (FPW), a byproduct of oil and gas production, contains modest concentrations (tens to hundreds of parts-per-million) of lithium, making it a potential resource. Among the various direct lithium extraction (DLE) approaches, the use of spinel lithium manganese oxide (LMO) ion-sieves for recovery of lithium from FPW stands out as one of the most promising materials due to their high lithium uptakes and rapid adsorption kinetics. However, LMOs can experience mass loss due to the reductive dissolution of manganese caused by high concentrations of free electrons in FPW, which impairs its recyclability. To address this issue, pristine LMO (Li1.6Mn1.6O4) was doped with 4 different concentrations of magnesium (Mg2+) to synthesize magnesium-doped lithium manganese oxides, Li1.6MgxMn1.6-xO4 or LMMO-x (where x = 0.1, 0.2, 0.3, 0.4). Lithium recovery tests in FPW show a 53% reduction in lithium uptake for LMMO-0.4 compared to pristine LMO, while the average manganese dissolution in the subsequent acid desorption was reduced by 80%. Cycling tests show that LMMOs retain 95% of their initial lithium uptake after the 5th cycle of use, compared to only 90% for LMO. These findings clearly demonstrate that LMMOs are more stable and exhibit better recyclability due to the magnesium doping. Extended X-ray absorption fine structure (EXAFS) analyses further confirm the improved stability of LMMOs, as irreversible structural contraction only occurred in LMO after 5 cycles of extraction. This study demonstrates that magnesium doping enhances the stability of LMMOs, making them promising candidates for lithium recovery from FPW.

11:20am - 11:40am, May 23
CPCE3: Evaluating the Mechanical performance of High-Frequency Induction Welded TRIP 690 (AHSS) tubes with Oxide inclusions
Sydney Okoroafor, University of Waterloo
Abstract: High-frequency induction welding (HFIW) is a well-established process for welding tubes and pipes for automotive and oil and gas applications, due to its high speed and low small weld sizes. This process has been recently used to weld new transformation induced plasticity (TRIP) steels for hydroformed automotive applications, which have been integrated into automotive design due to the ability of hydroformed TRIP steel parts to have thin-walls and high energy absorbing capabilities that both decrease vehicle weight and improve passenger safety while reducing vehicle CO2 emissions. However, due to the high alloying materials used in TRIP steels (particularly Al), welds in TRIP steels are prone to oxide inclusions thus narrowing the operating window to produce inclusion-free welds. Although it is accepted that these inclusions affect hydroforming performance, it is not known what bondline oxide content may be tolerated. The current study investigates how bondline oxides affect the bondline strength of HFIW TRIP 690 tubes. Bondline strength was measured using the ring hoop tensile tests (RHTT), a mechanical test where rings from tubes are loaded in the circumferential direction with fixtures that preserve the tubular geometry. These samples were taken from a batch of tubes with known...
oxide inclusions. As oxide distribution in the samples could not be controlled, an FEA model was created so that a more granular understanding of the relationship between HFIW strength and bondline oxide content could be had. This data enabled the development of a novel model relating bondline oxide inclusion coverage to tube bondline strength, as well it predicts the limit of the oxide coverage that may be tolerated without a loss in bondline strength.

11:40pm - 12:00pm, May 23
CPCE4: Crashworthiness of critical mineral-based high-entropy alloys designed for structural applications

Muyideen Adegbite, University of Calgary

Abstract: As the global commitment to energy transition grows, the use of clean nuclear energy is required to meet future energy and environmental demands, especially as the world’s population is likely to hit 10-billion people by 2050. It is posited that the current energy consumption and emission costs can be reduced by exploring the use of eco-friendly-nuclear energy generation systems, for which novel damage-tolerant materials are strategic to their launch, to improve safety and public confidence. From a metallurgical standpoint, there are a limited number of traditional alloys that can be optimized for the safe continuous operation of nuclear systems; as such, new high-performance damage-tolerant alloys such as high-entropy alloys (HEA) are rigorously and urgently sought. HEAs are a new class of alloys with four or more principal elements in nonequi- or equi-atomic proportion; they possess outstanding mechanical and functional properties compared to traditional alloys. This talk will first cover our efforts on the aggregation of mechanical data for several HEAs studied over a strain rate decade (10^-5 s^-1 to 10^5 s^-1). This effort helps to discover a gap that opens a new window of opportunity in the design of critical mineral-containing HEAs for damage-tolerant nuclear systems. Taking a cue from the energy transition needs and its strategic fusion with critical minerals—building blocks for a green economy, this talk will focus on the design, development, and crash-worthiness investigation of new critical mineral-based HEAs—X0.3CoCrFeNi (X=Al,Mn) tailored to withstand damage due to explosive events prevalent in nuclear-plants. The effect of composition and strain rate on the dynamic mechanical response (and prevalent deformation mechanisms) of these HEAs will be discussed.

12:00pm - 12:20pm, May 23
CPCE5: A Hybrid Rate Theory Model of Radiation-Induced Growth Including the Formation of Prismatic Vacancy Loops

Mahdi Mohsini, Queen’s University

Abstract: Components of nuclear power plants are subjected to extremely harsh conditions, which include the collision of high energy particles. This results in complex phenomena such as radiation-induced growth. Two dominant mechanisms have been used to model the progress of radiation-induced growth over the course of radiation: Diffusional Anisotropy Difference (DAD) and Self-Interstitial Cluster Diffusion (SCID). Although these models show agreement with the experimental measurements used for their calibration, their generalizability is lacking. One characteristic of these models is the absence of a mechanism to describe the formation of prismatic vacancy loops during radiation. In this work, we have meticulously formulated a Hybrid model that integrates the contributions of the two mechanisms. In addition, for the first time, the hybrid model includes the formation of prismatic vacancy loops, as the precursor of basal vacancy loops. The generalizability of the hybrid model and improvement in capturing the characteristics of the radiation-induced growth is demonstrated by fitting the model to 32 different sets of experimental measurements.

2:40pm - 3:00pm, May 23
CPCE7: (Invited) Industrial Scale Challenges to the Production of Battery-Grade Graphite to Meet the Exploding Demands of Electric Vehicles

Kamal Adham, Hatch Associates

Abstract: The exploding demand for battery-grade graphite, driven by the electric vehicle (EV) sector, has exposed the industrial challenges facing the natural and synthetic graphite industries to provide the requisite quality and quantity of supply. Summarizing a number of case studies highlighting the established and emerging innovations, this paper showcases the opportunities open to the graphite producers, as a critical component of the clean energy industry. Natural and synthetic graphite products are used as battery material in many applications. Natural graphite has formed inside the earth’s crust at a moderate temperature (750°C), but very slowly in millions of years. Mother nature’s feedstock (fossilized plants) have varied in physical and chemical properties, hence, giving a wide range of characteristics and impurities to the mined natural graphite around the world. The natural impurities present at the mines typically require multiple beneficiation steps to yield a salable natural graphite concentrate (~90% purity) which then requires purification to achieve the battery grade quality (~99.9% carbon content). Alternatively, synthetic graphite
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can be produced from purer feedstock (e.g. petroleum or coal coke) but requires ultra high temperature furnaces (~3,000°C) for the graphitization reactions to be completed within a reasonable time frame (days). The EV battery industry consumes a mix of natural and synthetic graphite, demanding industrial innovations on both fronts to meet the escalating demands of the clean-energy seeking societies.

3:00pm - 3:20pm, May 23
CPCE8: Improved Direct Lithium Extraction (DLE) Adsorbents for Lithium Extraction from Lithium Bearing Waters (LBWs)
Karthik Ramachandran Shivakumar, University of Alberta
Abstract: The demand for Lithium (Li) is projected to increase exponentially in the next decade. Direct Lithium Extraction (DLE) technologies applied to Li-bearing waters (LBWs), have potential to expand the Li resource base. Among these technologies, ion-exchange type DLE (i-DLE) materials have proven to be among the most effective in extracting Li from LBWs. Manganese (Mn) spinel type adsorbent are one of the i-DLE adsorbents that have high Li adsorption capacity and kinetics. One of the challenges associated with Mn adsorbents is Jahn-Teller distortion of the spinel during the extraction process. Furthermore, adsorbent loss through reductive dissolution of Mn caused by dissolved organic compounds and H2S present in LBW is another challenge for large-scale adaptation. By using material science approaches to study different surface modification and encapsulation methods, we propose techniques to mitigate the reductive dissolution of Mn spinel during the Li extraction process. Among the approaches tested, surface modification of the Mn spinel with a 7.5 nm layer of Zirconia reduced Mn loss by 50% in a field collected LBW from Clearwater, Alberta. In another approach, encapsulation of the Mn spinel in polymeric fibers reduced Mn loss by 95% in the same LBW. Experimental results show that the adsorption capacity of the Mn spinel is controlled by both the adsorbent particle size and the pH of the LBWs during reaction. Optimization of these two parameters successfully reduced Mn loss to approximately 0.5% after 16 cycles with Li uptake of 20 mg/g at 6 h of extraction time per cycle. Extended X-ray absorption fine structure (EXAFS) analysis showed no significant degradation of the Mn spinel after 16 cycles. Extrapolating the results, it is economically feasible to recycle the developed Li adsorbent for over 100 cycles. Our laboratory findings show that inhibiting the reductive dissolution of Mn makes Li extraction from LBWs containing elevated organic compound levels feasible.

3:20pm - 3:40pm, May 23
CPCE9: Improved Direct Lithium Extraction (DLE) Nanoscale Transport during Liquid Film Thinning Inhibits Bubble Coalescing Behavior in Electrolyte Solutions
Qingxia Liu, University of Alberta
Abstract: Our research demonstrates that the film thinning exhibits a rather sudden slowdown (at around 30–50 nm) in electrolyte solutions, which is quite different from the system involving surfactants. The difference in solute concentration between the bulk and the surface was attributed to this observed phenomenon. During film thinning, an electrolyte concentration difference in film solution along the interacting region causes a Marangoni stress to resist film thinning. The retarded film thinning between two bubbles and delayed bubble coalescence were quantitatively explained by the proposed electrolyte transportation at nanoscale. This finding clearly highlights the coupled effects of interfacial flow and ion specificity, which shows essential implications for improved understanding of ocean waves and future development of colloidal science in high concentration electrolyte solutions. The research offers a new insight for a better understanding of biology system and other applications such as water splitting and mineral extraction in high concentration electrolyte solutions.

4:00pm - 4:20pm, May 23
CPCE10: Improved Direct Lithium Extraction (DLE) Nanoscale Transport during Liquid Film Thinning Inhibits Bubble Coalescing Behavior in Electrolyte Solutions
Qingxia Liu, University of Alberta
Abstract: Our research demonstrates that the film thinning exhibits a rather sudden slowdown (at around 30–50 nm) in electrolyte solutions, which is quite different from the system involving surfactants. The difference in solute concentration between the bulk and the surface was attributed to this observed phenomenon. During film thinning, an electrolyte concentration difference in film solution along the interacting region causes a Marangoni stress to resist film thinning. The retarded film thinning between two bubbles and delayed bubble coalescence were quantitatively explained by the proposed electrolyte transportation at nanoscale. This finding clearly highlights the coupled effects of interfacial flow and ion specificity, which shows essential implications for improved understanding of ocean waves and future development of colloidal science in high concentration electrolyte solutions. The research offers a new insight for a better understanding of biology system and other applications such as water splitting and mineral extraction in high concentration electrolyte solutions.

4:20pm - 4:40pm, May 23
CPCE11: Influence of Metal-Ion Doping on Calcite Growth
Li Yue, University of Alberta
Abstract: Calcium carbonate (CaCO3) is one of the most abundant minerals in nature, which can be typically found in soil, water, and sedimentary rocks. Aside from the significance of this mineral in nature, the formation of water-scale deposits is one of the major issues in the industry. The development of scale layers could block the pipes and boilers, lower the efficiency of heating and cooling devices, and thus result in machine damage and production losses. Hence, CaCO3, especially the most stable polymorph calcite, has been a popular subject of extensive and varied studies. As the most common impurities in natural water environments, metallic ions are believed to be incorporated within the calcite lattice and inhibit the formation of water-scale deposits by retarding the growth of calcite crystals. To better understand the effect of metal-ion doping on the initial stage of calcite growth, the attachment of the CaCO3 molecule on hydrated pristine and doped (Mg-, Cu-, Zn-, Sr- and Ba-doped) calcite (10-14) surfaces and the analysis of the interactions of the water molecule with various doping ions were studied using the first-principles methods. Simulation results suggest that the adsorption behavior for water molecules is dominated by the chemical bonding, i.e., the stronger the water-dopant interaction, the less the adsorption energy. For the adsorption of the CaCO3 molecule on hydrated calcite surfaces, both the dopant size and the chemical bonding factors influence its stability, resulting in the decrease of the CaCO3 adsorption on all doped surfaces. By considering the synergetic effects of doping ions on the water and CaCO3 adsorption, we provide new insights into the understanding of the inhibiting mechanism of the Mg, Cu and Zn ions on calcite growth. This finding undoubtedly helps the industry develop effective and economical approaches to manage excessive calcite scaling issues.
**10:20am - 10:40am, May 23**
**MCMS1:** (Invited) Materials and Corrosion Management for a Sustainable Future

*Monica Hernandez, Infinity Growth Corp*

**Abstract:** This symposium is a pivotal forum that explores the intricate interplay between corrosion, integrity management, and sustainability. The symposium endeavors to catalyze a paradigm shift towards the adoption of a holistic approach to materials and corrosion management. This approach aims to mitigate failures, environmental incidents, and financial burdens while concurrently fostering the principles of a circular economy. Attendees are invited to engage in discussions and knowledge-sharing sessions, delving into innovative strategies and practices for achieving a sustainable future in materials and corrosion management.

**10:40am - 11:00am, May 23**
**MCMS2:** Effect of Hydrogen Absorption on Microstructural, Mechanical and Corrosion Properties of Aged Legacy Pipelines

*Akhilesh Reddy Chopra, The University of British Columbia*

**Abstract:** The migration of atomic hydrogen within pipeline steel microstructure can increase susceptibility to hydrogen embrittlement, posing metallurgical challenges for hydrogen pipeline transportation. This issue is exacerbated by the repurposing of legacy pipelines that have experienced metallurgical ageing throughout operational lifespan. The present study aims to evaluate the effect of hydrogen absorption on the microstructural, mechanical and corrosion properties of a decommissioned 1950s natural gas pipeline. Results were compared with API X65 modern pipeline steel. Mechanical testing of both sample groups established baseline conditions, with energy dispersive X-ray spectroscopy (EDS) used to detect manganese sulfide inclusions and assess anisotropic behavior. Hydrogen uptake capacity post full-scale ageing of the pipeline was evaluated, with insights into residual hydrogen loading obtained through LECO combustion and thermal desorption analysis. Hydrogen permeation studies using the Devanathan Stachurski method revealed a higher permeation rate in the legacy pipe due to its aged structure than in the X65 steel. Samples were also cathodically charged with hydrogen in 0.3M sulfuric acid over different charging intervals (4, 8, 12, 16, and 24 hours). Mechanical properties of hydrogen charged and uncharged legacy and X65 steel samples were compared. Thermal desorption analysis were used for hydrogen absorption quantification. Furthermore, electrochemical potentiodynamic polarization elucidated the corrosion behavior of hydrogen-adsorbed legacy pipelines compared to uncharged and charged modern steel, providing insights into changes in open-circuit potential and corrosion current density. Post-surface analysis employed optical microscopy, scanning electron microscopy, and X-ray diffraction. This study aims to deepen understanding of material degradation in legacy pipelines, possibly repurposed for hydrogen transport, to ensure long term safety and reliability.

**11:00am - 11:20am, May 23**
**MCMS3:** Fracture Toughness Mechanism in Girth Welded X70 Pipeline Steel with Different Ti/N Ratio

*Vanda Milani, University of Alberta*

**Abstract:** The fracture mechanism in girth-welded X70 pipeline steel with different Ti/N ratios was investigated. The ratios were 2.9, 3.9 and 5.1, representing hypo-stoichiometric (Hypo), near stoichiometric (Sto), and hyper-stoichiometric (Hyper), respectively. The welding technique used was shielded metal arc welding (SMAW). The crack tip opening displacement (CTOD) toughness for the tested specimens were 0.65, 0.34, and 0.07 mm for the Hyper, Sto, and Hypo, respectively. The cleavage fracture facet size was observed to be the largest for the Hypo sample. A significant difference in the total number of M-A between samples was measured. The total number of M-A for the Hypo, Hyper, and Sto were approximately 0.08, 0.05, and 0.03 per µm 2 for the 315 µm scanned area, respectively. The result shows that CTOD fracture toughness increases with an increasing Ti/N ratio. This increase is mainly attributed to the decrease in PAG and the M-A area fraction.

**11:40am – 12:00pm, May 23**
**MCMS 4:** (invited) Investigating the Behaviour of Welded Joints in a High Toughness Naval Steel Under Different Strain Conditions

*Alison Mark, Defence Research and Development of Canada*

**Abstract:** Welded joints can be a weak point in a boat’s construction. It is important to qualify the welds for performance in ‘real’ conditions, which include long-term use and ‘abuse’ (deformation), and to understand their evolving material properties. Having the correct data to carry out calculations to predict material behaviour - will it deform, crack, fail; will a crack grow; how fast - is important for informed repair and maintenance. It is generally better for both budgets and the environment to replace when possible. This presentation will report on results from a variety of tests carried out on welded joints in a high toughness naval steel. The mechanical properties of the base metal and the weld metal “as built” will be presented, as will the effects of prior strain on tensile properties, fracture toughness and fatigue crack growth rate. The mismatched properties across the joints and high strain rate cracking behaviour will be explored.
For the base metal, both strength and fracture initiation toughness increased with pre-strain up to 9%, the latter being unexpected; pre-strain had a minimal effect on fatigue crack growth rate. The welds were designed to have matching strength to the base metal; tensile tests on base metal, weld metal and cross-weld coupons indicated that the strengths were within 2%. Nonetheless, weld-base metal mismatch was evident in straining and cracking behaviour of specimens with full weld joints at quasistatic and high strain rates. Preliminary thoughts on mechanisms and future work arising from this study will be discussed.

**12:00pm – 12:20pm, May 23**

**MCMS5: Effect of Electrochemical Hydrogen-Charging Conditions on Nanomechanical Properties of X80 Pipeline Steel**

_Qing Hu, University of Calgary_

**Abstract:** In this work, nanoindentation tests, combined with electrochemical hydrogen (H)-permeation testing, were used to study the effect of H-charging conditions on H-permeating parameters and nanomechanical properties of X80 pipeline steel. The H-charging environment and condition remarkably affect the H-permeating parameters. The steady-state H-permeating current density, H-permeating flux, and the H subsurface concentration obtained in 0.5 M H2SO4 solution are apparently greater than the parameters obtained in near-neutral pH NS4 and 0.1 M NaOH solutions. The nanomechanical properties of X80 steel are heavily dependent on H-charging and the charging conditions (i.e., solution, time, and cathodic current density). Under the open circuit state, the nanomechanical properties of pipeline steel are mainly affected by the anodic reaction in different electrolytes. In acidic environments, the mechanical properties continuously deteriorate, while in neutral and alkaline environments, due to the protective effect of corrosion product films, the mechanical properties first decrease and then increase. During the cathodic charging process, any factors causing an increase in H atom concentration in the steel, such as increased H-charging time, application of a cathodic polarization current density and conduction of H-charging in an acidic solution, lead to hardening of the steel. The evolution of the sample surface leads to a degradation in the reduced modulus.

**12:20pm – 12:40pm, May 23**

**MCMS 6: Corrosion Management of Bunsen Reaction for Sustainable Hydrogen Production from H2S Splitting Cycle and S-I Water Splitting Cycle**

_Xiaoling Li, University of Saskatchewan_

**Abstract:** Bunsen reaction is the centre one of those that form the hydrogen sulfide (H2S) splitting cycle and the Sulfur-Iodine (S-I) water splitting cycle, which lead to net hydrogen production from H2S and water, respectively. Both cycles can make hydrogen production and fossil fuel processing more sustainable. However, Corrosion management is pivotal not only to the Bunsen reaction but also to the entire cycles because very corrosive substances are involved in the reactions.

Both the reactants, sulfur dioxide (SO2), iodine (I2), and water (H2O), and the products, sulfuric acid (H2SO4) and hydroiodic acid (HI), of the Bunsen reaction are very corrosive, especially at the reaction temperature that is above the melting point of solid iodine. Materials are difficult to be found when machining the large-scale reactors for this reaction. By dissolving the iodine in a solvent to keep it flowable below its melting point, we lowered the Bunsen reaction temperature to ambient levels, under which the corrosion rate of the Bunsen reactants and product acids becomes low. The application of the Corning Advanced-Flow Reactors (AFR) for the multiphase Bunsen reaction not only enhances the mass transfer efficiency among phases but also their inorganic materials have totally prevented the acid corrosion from occurring. We will report the results of the quantified corrosion behavior of the Bunsen fluids (reactants and products) to the Corning AFR materials at ambient temperatures.

**2:00pm – 3:00 pm, May 23**

**MCMS7: Investigating Mechanical Properties of ARMOX 500T in High Strain Rates Using Direct Impact Hopkinson Pressure Bar: A Computational Study**

_Mohammad Mahdi Ghadiri, York University_

**Abstract:** High strength materials have been the subject of many researches in the past few decades, especially to investigate their response to high strain rates. Due to the high cost of such materials and considering the advancements in computational tools, numerical simulations can be utilized to improve the cost efficiency for analyzing the mechanical behavior of these materials. In this regard, Direct Impact Hopkinson Pressure Bar (DIHPB) machine is usually being used to determine the effect of high strain rates on the mechanical response of materials. Therefore, the main aim in this research is to provide a model for DIHPB machines to obtain the strength and failure strain of ARMOX 500T in a strain rate range of 1000 s-1 to 3000 s-1. Different material models such as Johnson-Cook and Zerilli-Armstrong will be used for ARMOX 500T to evaluate the efficiency of the models in high strain rates. The flow curves and failure strains obtained in each case will be compared to the experimental results from the literature.

**3:00pm – 3:20 pm, May 23**

**MCMS 8: Machine Learning Applications for Predicting Corrosion in Extreme Environments**

_Emilie Seto, University of Alberta_

**Abstract:** Current corrosion experiments are often material and time-intensive which limits the number of feasible experiments. Machine learning (ML) provides a solution to this challenge by employing algorithms capable of leveraging existing corrosion data to predict and identify patterns in the corrosion environment. Over the past decade, numerous ML applications in corrosion have emerged, showcasing the dynamic growth of this interdisciplinary field. These applications include predicting corrosion severity and rates for atmospheric corrosion and corrosion in the presence of inhibitors, oxidation kinetics, and visual corrosion detection.
Despite these advancements, the full spectrum of future applications and limitations in this emerging field is yet to be realised. Corrosion experiments in extreme environments, such as high-temperature and high-pressure applications, are notably resource-intensive and costly. The application of ML for corrosion severity prediction in these extreme environments presents an opportunity to streamline costs while providing invaluable insights into general corrosion patterns and areas of interest. This presentation will specifically explore the application of ML in two extreme corrosion environments: supercritical CO2 transportation and hot oxidation. Multiple ML models are investigated to identify the one with the highest accuracy for each environment. Additionally, the presentation will delve into the limitations and potential future applications of this methodology.

**3:20pm – 3:40pm, May 23**
**MCMS9: An Interatomic Potential for Sodium and Chlorine in both Neutral and Ionic States**
**Hao Sun, Queen's University**

**Abstract:** Molten salts can be the game-changing storage solution for liquid metal batteries and solar- or nuclear-generated heat. However, the central issue limiting their wide-spread application—corrosion to metallic containers—remains poorly under-stood. This knowledge gap necessitates fundamental atom-scale studies of molten salts. Using a small-cell active learning approach, we generate a moment tensor potential (MTP) trained on only 609 configurations, jointly describing solid/liquid Na, gaseous Cl, and crystalline/molten NaCl. This MTP implicitly captures the effect of atomic charge variations on energies and forces based on local atomic configurations. Extensive testing of this potential points to a high-fidelity description of the structural and transport properties of liquid Na and molten NaCl. Furthermore, this potential was used to calculate the standard reduction potential and solubility limit of Na in molten NaCl. These computed properties are in good agreement with available experimental data and ab initio calculations. Our proposed approach can be utilized to investigate the electrochemical and physical properties of molten salts with arbitrary compositions and solutes, as well as the molten salt corrosion of metals.

**4:00pm - 4:20pm, May 23**
**MCMS10: Hydrogen Embrittlement Susceptibility Assessment of Quenched and Tempered Casing Steel**
**Xu Zheng, McGill University**

**Abstract:** Hydrogen embrittlement (HE) of steel pipelines in high-pressure gaseous environments is a potential threat to the pipeline integrity. The occurrence of gaseous HE is subjected to associative adsorption of hydrogen molecules (H2) at specific “active sites” such as grain boundaries and dislocations on the steel surface to generate hydrogen atoms (H). Non-metallic inclusions are another type of metallurgical defects potentially serving as the “active sites” to cause the H2 dissociative adsorption. Al2O3 is a common inclusion contained in pipeline steels. In this work, the dissociative adsorption of hydrogen at the α-Al2O3 (0001)/α-Fe(111) interface was studied by density functional theory calculations. The impact of gas components of O2 and CH4 on the hydrogen dissociative adsorption was determined. The occurrence of hydrogen dissociative adsorption at the Al2O3 inclusion/Fe interface is favored under conditions relevant to pipeline operation. The thermodynamic feasibility is observed for Fe and O atoms but is not observed for Al atoms. H atoms can form more stable adsorption configurations on the Fe side of the interface, while it is less likely for H atoms to adsorb on the Al2O3 side. There is a greater tendency for the occurrence of dissociative adsorption of O2 and CH4 than H2 due to their more favorable energetics. Particularly, the dissociative adsorption of O2 is more preferential over CH4. The Al-terminated interface exhibits a higher H-binding energy compared to the O-terminated interface, indicating a preference for hydrogen accumulation at the Al-termination of the interface.

**4:40pm – 5:00pm, May 23**
**MCMS 12: The effect of Ti/N ratio on the microstructure of the inter-critically reheated heat affected zone for a multi-pass X70 steel girth weld**
**Vanda Milani, University of Alberta**

**Abstract:** The effect of the Ti/N ratio on the microstructure of the inter-critically reheated coarse grain heat affected zone (ICCGHAZ) for a multi-pass X70 girth weld was studied. Three different X70 steels with a Ti/N ratio of 2.4 (hypo-stoichiometric: Hypo), 3.3 (stoichiometric: Sto), and 5.1 (hyper-stoichiometric: Hyper) were welded using shielded metal arc welding (SMAW). The mean size/volume fraction ratio of (Ti,
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(Nb)(C, N) precipitates. The ratio was intermediate for the Sto specimen (3.83x10^4 nm). The prior austenite grain (PAG) sizes for the IC&GHAZ were 27.0, 37.2 and 50.6 µm for the Hyper, Sto and Hypo samples, respectively. The results show that PAG size in the IC&GHAZ increases with decreasing Ti/N ratio. This is attributed to an increase in the mean size and a decrease in the volume fraction of (Ti, Nb)(C, N) precipitates.

10:00am – 10:20pm, May 24
MCMS 14: Development of CoCrNi Medium Entropy Alloy Against Hydrogen Embrittlement
Hanifeh Ahmadi, University of Alberta
Abstract: Hydrogen embrittlement is a major issue in various industries where components are exposed to hydrogen, such as nuclear hydrogen production reactors operating under extreme conditions. Hydrogen embrittlement is a reduction in the ductility of a metal, because hydrogen atoms are small and can penetrate metal microstructures, lowering the stress needed to initiate and propagate cracks in the metal. Traditional alloys such as stainless steel 316 can fail due to hydrogen embrittlement which limits their performance in hydrogen-rich environments. A new generation of materials known as High/Medium Entropy Alloys (HEA/MEAs) have shown promising properties (e.g., good resistance to wear and corrosion) to deal with hydrogen embrittlement and consequent failure. These alloys, made up of more than five elements in roughly equal proportions, offer outstanding properties like high strength, high tensile ductility and high fracture toughness, particularly at cryogenic temperatures. As a result, they are promising candidates to be used in energy-related applications like hydrogen tanks and nuclear devices. This presentation will explore the characterization of CoCrNi MEA produced by vacuum arc re-melting (VAR), specifically examining their resistance to hydrogen embrittlement. We will discuss the underlying mechanisms that contribute to their resistance to hydrogen embrittlement.

10:20am – 10:40pm, May 24
MCMS 15: Pin-on-disc wear behaviours of CoCrNi and FeCoNi medium-entropy alloys up to 1000 °C
Wandong Wang, University of Toronto
Abstract: The FeCoNi and CoCrNi alloys prepared via the arc-melting method were investigated for their microstructure and high-temperature wear performance. The tribological tests were conducted in a pin-on-disc configuration with an alumina ball as a counter-surface at a wide range of temperatures (25-1000 °C). Scanning electron microscopy (SEM) equipped with energy-dispersive X-ray spectroscopy (EDS) was used to analyze the worn surfaces, wear debris, and alumina balls. Raman spectroscopy was employed to characterize the tribo-oxide layer formed on the samples. FeCoNi medium-entropy alloy (MEA) exhibited excellent resistance to wear at ambient temperature (8.5×10^-6 mm3/Nm) due to the formation of a tribo-oxidized layer while its resistance deteriorated quickly with increasing temperature. Once the dense glaze layer formed at 800 °C, the resistance increased. CoCrNi MEA exhibited a relatively higher volume loss at ambient and intermediate temperatures because of the large adhesion force between the alumina balls and the testing surface. CoCrNi exhibited a better oxidation resistance compared to FeCoNi due to high Cr content postponing the severe-mild transition to a higher temperature (1000 °C). This study demonstrated the effect of compositions and oxidation on the wear performance in MEAs.

10:40pm – 11:00am, May 24
MCMS 16: Interfacial Segregation and Adhesion Effects in Equiatomic CoCrFeNi High Entropy Alloy
Dennis Boakye, University of Manitoba
Abstract: First-principles density functional theory (DFT) is employed to investigate the role of reactive elements, specifically Hafnium (Hf) and Yttrium (Y), in enhancing the oxidation resistance of equiatomic CoCrFeNi high-entropy alloy (HEA). Experimental evidence suggests that these elements function as sulfur-getters in high-temperature applications but do not completely pin sulfur within the bulk, prompting a detailed exploration of interfacial segregation and its implications on the metal-oxide interface. Our findings reveal that both Hf and Y effectively immobilize sulfur within the bulk through the formation of robust ionic bonds, featuring a notable covalent character. Comparative analysis indicates that the segregation of Y and Hf enhances interfacial plasticity, while sulfur segregation weakens and embrittles the interface substantiating the so-called "Sulfur effect". Interestingly, Hf has a more pronounced effect on interfacial adhesion, while Y is more effective in sulfur pinning. Co-segregation of Hf and Y with unpinned sulfur mitigates the deleterious effects, showcasing potential for improved scale adhesion in HEAs. This research provides valuable insights into mechanisms governing the interplay between reactive elements and sulfur, offering a foundation for designing advanced materials with enhanced high-temperature performance.
10:00am - 10:20am, May 24
MACC1: Effect of PH and Stirring Rate on Micro-Indentation Hardness and Microstructure of Ni-SiO$_2$ Nanocomposite Coatings Electrodeposited from Deep Eutectic Solvent
Mehry Fattah, York University
Abstract: In this work the effect of the electrolyte PH and stirring rate on microstructure and micro indentation hardness of Ni-SiO$_2$ nanocomposite coatings electrodeposited from an environmentally friendly deep eutectic solvent (DES) containing 30 g/L of SiO$_2$ nano powder (5-20 nm) was investigated. A choline chloride/ethylene glycol-based DES electrolyte was used for the electrodeposition at constant current density of 8 mA cm$^{-2}$ and different stirring rates of 600, 800, and 1000 rpm for 90 min. Acid boric was used to balance PH of the electrolyte around 3 and 5. Microstructure, composition, and hardness measurements were evaluated employing scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDX), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and micro indentation hardness measurements. Zeta potential of SiO$_2$ nano powder in the electrolyte were measured using zeta sizer machine. Nano crystalline Ni coatings with the same crystallographic planes were detected for the Ni-SiO$_2$ coatings. However, Ni clusters’ size increased remarkably with the decrease of stirring rate from 1000 to 600 rpm. The amount of SiO$_2$ content in the coatings increased from 0.56 wt.% and 4.1 wt.% (measured using EDX and XPS, respectively) up to 6 wt.% (measured point obtained through experiments, and the phase using EDX) with the decrease of stirring rate from 1000 to 800 rpm and PH of the electrolyte from 5 to 3. This can be related to the more positive zeta potential of SiO$_2$ nanoparticles in the presence of acid boric (PH=3) and more attraction of the particles to the cathode surface leading to the higher number of adsorbed particles in the growing Ni matrix during electrodeposition. This behavior resulted in the increase of the cross-section hardness values from 520 ± 20 Hv10gf up to 600 ± 20 Hv10gf, due to the higher amount of SiO$_2$ nanoparticles in the Ni matrix and more barrier against dislocation movement based on dislocation and dispersion hardening mechanism.

10:20am - 10:40am, May 24
MACC2: Step load nanoindentation: physical model and comparative study on FCC systems
Lizhong Lang, University of Toronto
Abstract: Step load method facilitates nanoindentation tests at high strain rate up to 10$^{4}$ s$^{-1}$, making it possible to study microscale shock and impact mechanics on surface coating. Yet it still suffers from issues with dynamic calibration and data processing: The scattering nature of second order derivatives of acceleration prevents precise calibration of load, and there is no reliable physical model describing the constitutive relation in high strain rate nanoindentations. This work proposed a physical model leading to a constitutive relation in the form of an ordinary differential equation, the numerical solution of which fits well with data collected from FCC metals (Cu, Ni) and alloys (NiCo). The influence of alloying elements and crystal orientation on high strain rate indentation was studied compared by the modified step load method.

10:40am - 11:00am, May 24
MACC3: Mechanical Behavior of AlCoCrFeMo High-entropy Alloy under Uniaxial Tension using Molecular Dynamics Simulation
Nashit Jalal, University of Alberta
Abstract: High-entropy alloys (HEAs) have emerged as a novel category of advanced metallic materials, attracting considerable interest. This class of alloys presents a distinctive blend of mechanical, thermal, and functional properties, rendering them well-suited for a diverse range of industrial coating applications. Among these alloys, the equi-atomic body-centered cubic (BCC) phase AlCoCrFeMo stands out as a recently developed composition with promising attributes for various engineering applications. In this study, the mechanical behavior of the AlCoCrFeMo high-entropy alloy under uniaxial tensile loading is studied using atomistic simulation to investigate the effect of Mo concentration on the yield strength and elasticity of the alloy. The model was validated using the lattice parameter and melting point obtained through experiments, and the phase stability was studied using polyhedral template matching (PTM). We observed an increase in the strength and elasticity of AlCoCrFeMo alloy as a function of increase in Mo concentration. The chemical short-range ordering was also quantified using the Warren-Cowley parameter and no significant correlation between short-range ordering or local lattice distortion and Mo concentration was observed. Lastly, the calculation of the atomic strain showed the formation of bands with high shear strain after the yield point. The formation of shear bands was used to explain the deformation mechanism exhibited by the alloy system: the localized strain acts as a softening mechanism during plastic deformation. The findings obtained from this investigation indicate that by adjusting the concentration of Mo, the mechanical properties of the AlCoCrFeMo alloy can be tailored, providing new opportunities for developing functional coating materials.
Keywords: High-entropy Alloy (HEA), Molecular Dynamics, Polyhedral Template Matching, Shear Bands, Short-range Ordering
**MACC4:** Hardness of Cold-sprayed Stable Nanocrystalline High-Entropy Alloys Evaluated through Nanoindentation

Kasimuthumani Subramanian, University of Calgary

**Abstract:** Surfaces of metallic components intended for engineering applications, including automobile engines, turbine blades, and aerospace parts, are often exposed to extremely corrosive, abrasive, and oxidative environments during their service lifetime. Such exposure wears the machine parts and results in premature failure of the entire engineering system or extra costs associated with maintenance and replacement of the worn parts. To reduce the impact of wear, hard and corrosion-resistant coatings are often applied to protect the underlying substrate from the aforementioned degradation mechanisms. Here, we report the mechanical properties and structure of an ultra-high strength, wear-resistant, and lightweight multifunctional metallic coating deposited on a steel substrate through a cold-spray process. These coatings were developed from stable nanocrystalline (NC) high-entropy alloy (HEA) powders that possess superior mechanical, wear, and corrosion resistance properties. More specifically, two NC-HEAs films of approximately 8 µm thickness deposited on A36 carbon steel were examined: Al25Co25Cr25Fe25 (undoped) and Al24.6Co24.6Cr24.6Fe24.6Zr1.5 (doped). Further, the impact of post-deposition heat treatment on the mechanical properties of the coatings was examined through nanoindentation: the as-deposited coatings and coatings that were heat treated at 873 K. We observed that the hardness of the coatings for both heat treatments was almost 3 times more than the hardness of the substrate. Further, the heat-treated coatings exhibited an improvement of approximately 20 percent in hardness and elastic modulus compared to the as-deposited HEA coatings. Additionally, examination of the indents using atomic force microscopy (AFM) and transmission electron microscopy (TEM) allowed for the identification of the deformation mechanisms responsible for the changes in the hardness. Overall, these results demonstrate an important step toward the design of multifunctional lightweight metallic coatings for sustainable energy generation systems in cold climates.

**MACC6:** (Invited) Submerged-Arc Welding Overlay for impact abrasion applications

Jing Li, Trimay Wear Plate Ltd.

**Abstract:** Overlay materials have been widely used in various industries such as oil and gas, mining, agriculture, asphalt, and forestry. Iron-based overlay materials, produced through the welding processes, provide feasible and economical overlay material production. In application environments, aside from typical sliding abrasion, complex wear conditions are often encountered, such as corrosion-abrasion and impact-abrasion. In this work, a welding overlay material is reported for impact abrasion applications. A submerged arc welding process has been employed to prepare the overlay. Optical microscope and scanning electron microscope images show that the overlay exhibits a hypereutectic microstructure containing multiple primary hard phases within an austenitic/martensitic matrix. Microhardness, ASTM G65 procedure A, and impact abrasion tests have been performed to examine the overlay. The material has shown less wear loss in the rotary impact test than other commercially available chromium carbide overlays.

**MACC5:** Effect of Al-Si coating weight on the experimental heat transfer coefficient of 22MnB5 steel during hot stamping

Ardhendu Bhattacharya, University of Waterloo

**Abstract:** Automotive manufacturers are increasingly using ultra-high strength steel to manufacture body-in-white components through hot stamping to reduce vehicle weight while retaining crashworthiness. A common steel grade used in hot stamping is 22MnB5 coated with a ~90-10 wt. % Al-Si coating. The coating protects against corrosion and prevents oxidation and decarburization during austenitization. Many hot stamped parts, however, are scrapped due to the formation of softer steel phases such as ferrite and bainite during the process. The formation of fully martensitic parts during hot stamping is contingent on the interfacial heat transfer coefficient (HTC) between the blank and the tool. Therefore, it is critical to understand the effects of different process parameters on the heat transfer between the blank and die for hot stamping practitioners in the industry. This work looks at the effect of the Al-Si coating weight on the experimental HTC during hot stamping. Blanks with two different coating weights were hot stamped at varying interfacial pressures and blank and die temperatures were measured in situ. The HTC was derived by inverting subsurface temperature measurements of the die during hot stamping experiments using inverse heat conduction analysis. Experimental HTCs were compared between the two coating weights to characterize the effects of coating weight on the HTC. Roughness and microhardness measurements of the blanks out of the furnace were collected to correlate surface states after austenitization to the HTCs.

**MACC7:** (Invited) Submerged-Arc Welding Overlay for impact abrasion applications

Jing Li, Trimay Wear Plate Ltd.

**Abstract:** Overlay materials have been widely used in various industries such as oil and gas, mining, agriculture, asphalt, and forestry. Iron-based overlay materials, produced through the welding processes, provide feasible and economical overlay material production. In application environments, aside from typical sliding abrasion, complex wear conditions are often encountered, such as corrosion-abrasion and impact-abrasion. In this work, a welding overlay material is reported for impact abrasion applications. A submerged arc welding process has been employed to...
prepare the overlay. Optical microscope and scanning electron microscope images show that the overlay exhibits a hypereutectic microstructure containing multiple primary hard phases within an austenitic/martensitic matrix. Microhardness, ASTM G65 procedure A, and impact abrasion tests have been performed to examine the overlay. The material has shown less wear loss in the rotary impact test than other commercially available chromium carbide overlays.

02:00pm - 02:20pm, May 24
MACC8: A “gene-like” parameter for material tailoring: Begin with the electron work function for multi-element carbide discovery—A first-principles study
Dong Zhang, University of Alberta
Abstract: Metal carbides are widely used in wear-resistant materials and protective coatings. Metal doping or substitution influences the strengths of covalent, ionic, and metallic bonds as well as their distribution in carbide’s structure, thereby altering mechanical properties of the carbide. Multi-element carbides have attracted increasing attention due to their modifiable properties. However, designing multi-element carbides and selecting metal substitutes or dopants for developing advanced carbides need effective guidelines in order to minimize trial-and-error experiments. Electron work function (EWF) has been demonstrated to be a promising variable or an effective indicator similar to encoded parameter carrying material “genetic” information for guiding dopant or substitute selection. The higher the carbide's EWF, the higher its bulk and Young’s moduli. Since EWF can reflect synergistic influence of various factors, e.g., net charge, bond order, electron localization function and energy states, on mechanical properties of carbides, incorporating EWF into machine learning models has shown improved bulk and Young’s moduli prediction. In this talk, the role of EWF in guiding carbide design and modification will be demonstrated and discussed.

02:20pm - 02:40pm, May 24
MACCS: Cold Sprayed De-Icing Coating: Techno-Economic Assessment
Peter Menghesha, University of Alberta
Abstract: Design, manufacturing, and usage of efficient heating systems for pipelines and closed pressure equipment are necessary for cold regions to compensate for heat loss and prevent damage caused by freezing of the enclosed liquid. Given large-scale financial losses stemming from failure and bursting of the pipes, development of novel, efficient, and affordable heaters with environmental benefits is of crucial importance. Heating systems have already been produced via different high-temperature thermal spraying techniques to achieve higher efficiency compared to conventional heating cables. In this study, tin, as the heating element, was deposited using the cold spray process onto alumina and alumina-titania dielectric coatings that were fabricated by flame spraying (FS) to provide electrical insulation. A techno-economic assessment of fabrication and utilization of the coating-based heaters was conducted. It was found that cold-sprayed heater coatings exhibit improved performance and economic feasibility compared to other thermally sprayed heater coatings and conventional heater cables. The results suggest that the new generation of coating-based heating systems may be competitive with conventional heat tracers that are widely used in industry.

02:40pm - 03:00pm, May 24
MACC10: Correlations between the radiometric properties of galvanneal coating and its phase composition and surface topology
Michiyko Kagaya, University of Waterloo
Abstract: Galvannealed steel automotive-grade is produced by heating zinc-coated steels, yielding an intermetallic zinc-iron coating having excellent corrosion resistance, as well as good paintability and weldability, provided the correct intermetallic phases are formed. This, in turn, requires precise temperature control and is crucial for quality control and efficiency improvement. Currently, pyrometry is commonly used across industry; however, accurate pyrometry hinges on knowing the radiometric properties of the galvannealed steel, but these are presently uncertain and vary with process parameters, alloy composition, and the composition of the zinc bath. This study aims to fill this knowledge gap by correlating the phase composition and surface topology of the galvannealed coating with its radiometric properties. The radiometric properties are determined using Fourier Transform Infrared Spectrometry (FTIR), X-ray Energy Dispersive Spectroscopy (EDS), and a digital microscope. The correlations found through this study may then be used to develop a physics-based model. Since the phases present in the galvanneal coating change during the heating process, the findings of this study may also potentially aid in improving the online pyrometry of galvannealed steel.

03:20pm - 03:40pm, May 24
MACC11: Cold Sprayed Al-Based High Entropy Alloy Coatings with Zirconium Dispersoids
Mohammad Aatif Qazi, University of Alberta
Abstract: High entropy alloys (HEAs), derived from equiatomic combinations of five or more elements, exhibit exceptional mechanical properties due to their solid solution structures. In particular, thermal-sprayed HEA coatings based on AlCoCrFeMo were recently found to exhibit exceptional mechanical properties compared to common industrial steel. In this study, the effect of 5 wt. %, 10 wt. %, and 15 wt.% addition of Zr on the hardness and erosion resistance properties of AlCoCrFeMo HEA coatings was investigated. The coatings were deposited on a 316 steel substrate using the cold spray technique, followed by subsequent heat treatment for phase stabilization. The spray parameters, including stand-off distance and traverse speed, were optimized to achieve a well-adhered coating to the substrate. The coating microstructure was characterized using a scanning electron microscope (SEM) and the...
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phase formation was determined using X-ray diffraction (XRD). Microhardness testing and solid particle impingement erosion testing based on a modified ASTM Standard G76 protocol were conducted to assess coating performance. Phase analysis of the fabricated coatings revealed the presence of body-centered cubic (BCC) phases. Microhardness measurements revealed that the coatings with Zr demonstrated superior hardness compared to the base AlCoCrFeMo coating and the uncoated substrate. Overall, the results suggest that cold-sprayed HEA coatings have potential as durable and erosion-resistant solutions for protecting industrial components in harsh environments.

03:40pm - 04:00pm, May 24
MACC12: Self-stable Nanocrystalline High-Entropy Alloy for High-performance Metallic Coatings
Moses Adaan-Nyiak, University of Calgary
Abstract: Grain coarsening is ubiquitous in nanocrystalline (NC) materials at low homologous temperatures, thus limiting their engineering applications, including surface coatings. Alloying with an extra solute-element to effectively offset the excess energy at the grain boundaries (GBs) of a principal element, which is the driving force for grain growth, is one established pathway to circumvent the thermal instability in binary alloy systems. However, this strategy is judged to be complex for multi-element alloys like high-entropy alloys (HEAs) because of the many pairwise interactions that exist among the constituent elements that may favor the formation of deleterious second phases. In this work, we show for the first time that nanograins in multi-element HEAs can self-stabilize without solute-element addition if one or more constituent elements of the HEA with the highest enthalpy of mixing and melting point segregate and decorate the GBs; this is termed self-stabilization in HEAs. Using AlCoCrFe as a model HEA, in-situ XRD, S/TEM, and atom probe tomography (APT) analyses show that Cr and Fe segregate at GBs by site-competition to stabilize ~9 nm-sized grains at 0.5Tm (Tm-melting temperature). GB desegregation that precedes phase decomposition sets on at 0.6Tm. The NC-AlCoCrFe HEA exhibits improved nanograin stability when compared with other NC-HEAs in the literature. Despite being in a nanocrystalline state, cold-sprayed NC-AlCoCrFe HEA shows evidence of metallurgical bonding at the particle-substrate and particle-particle interfaces—this opens a new window for designing lightweight ultra-high-strength wear-resistant metallic coatings on surfaces operating in low and high-temperature environments.

04:00pm - 04:20pm, May 24
MACC13: Effects of Chain Configuration and Stoichiometry on the Behavior of Boron Carbide at Elevated Temperature from First Principles Quasi-harmonic Approach
Sara Sheikh, University of Alberta
Abstract: Boron carbide, an advanced ceramic, exhibits high chemical and thermal stability, high hardness and strength, and abrasion and wear resistance. In this study a quasi-harmonic approach composed of static calculations from density functional theory and phonon theory within density functional perturbation theory is employed. This allows for the prediction of lattice structural changes with temperature which affect the elastic and thermal properties of the material. Temperature-dependent C_ij thermal expansion coefficient (TEC), Helmholtz free energy, entropy, and heat capacity at constant volume (C_v) of boron carbides with different carbon concentrations, chain configurations, and stoichiometries have been predicted using first principles quasi-harmonic phonon calculations. A good agreement between elastic constants and structural parameters from static calculations is observed. The trend in the temperature-dependent thermal expansion coefficient (TEC) reveals a minor increase below 100K, followed by a rapid rise up to 500-700K, and then a gradual increase towards a nearly constant value. This pattern is attributed to the transition from internal energy dominance to vibrational entropy dominance, indicating significant changes in the material’s behavior as temperature increases. Temperature-dependent C_ij s values are predicted, enabling stress analysis at elevated temperatures. The distinction of C_44 trend with temperature highlights boron carbide’s anisotropic behavior. Overall, the findings of this study can be used to perform mechanical and thermal stress analysis and optimize the design of boron carbide materials for elevated temperature applications.

04:20pm - 04:40pm, May 24
MACC14: Influence of processing parameters on mechanical properties of layer-cladded Inconel 718
Junteng Yuan, China University of Mining and Technology
Abstract: Studying the microstructure and macroscopic properties of coatings with different processing parameters by laser cladding is important for enhancing their overall performance, including hardness and strength, and for extending service life of coatings. In this study, IN718 coatings were prepared by laser cladding. The effects of processing parameters such as laser power P, scanning speed F, and powder feeding rate S on the microstructure and mechanical properties of IN718 coatings were investigated. As Nb element segregation and the Laves phase increase, the microhardness gradually reduces. It was discovered in the study within the range of processing parameters that with the increase of laser energy input, the microhardness, yield strength, and tensile strength of the cladding layer increased, while the elongation decreased. The tensile fracture mechanism of the coating is mainly plastic fracture, with a small amount of brittle fracture. Small and many fracture dimples cause the coating to have excellent tensile strength but low ductility.
**Abstract Appendix**

<table>
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<th>Time</th>
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<th>Symposium: Metal-Additive-Manufacturing: Processing, Structure, and Properties (MAMP)</th>
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| 10:00am - 10:20am | MAMP1: (Invited) Extreme mechanics, materials, and manufacturing across scales | Yu Zou, University of Toronto  
**Abstract:** Many of today’s most critical infrastructure and machinery (for example, next-generation turbines, mineral exploration equipment, nuclear reactors, and critical medical implants) are made with materials that operate under extreme conditions. Innovations in material development and manufacturing processes for such demanding conditions are necessary and urgent to increase the service life of existing infrastructure and to open the door to new applications. Towards this vision, my presentation will focus on the exploration of mechanical behavior and manufacturing processes of materials across many length- and time-scales. I will first introduce our recently developed versatile in situ electric field. Then, I will share insights on the recent work on controlling dislocation motion using an electric field. I am also going to talk about our recent work on controlling dislocation motion using an electric field. Then, I will share insights on the recent work on controlling dislocation motion using an electric field. 

**Abstract:** This study investigates the application of laser rescanning as a post-process heat treatment to enhance product quality during Laser Powder Bed Fusion. Focusing on Al-Si-based alloys, a 3D Cellular Automata (CA) simulation of grain structure is coupled with a Finite Element Analysis of temperature evolution to simulate microstructure evolution during the LPBF laser rescanning process. Various scanning strategies are explored to assess their effects on grain structure refinement and texture (crystallographic orientation). Our findings reveal that altering scanning directions during laser rescanning, such as bi-directional and island scanning, leads to more significant grain refinement as compared to uni-directional scanning. The enhanced grain refinement is seen to be a result of the variations in heat flux and the occurrence of repeated thermal circles as the laser changes scanning direction. Furthermore, these strategies are seen to substantially modify both the overall and localized crystallographic textures. Varying scanning directions during rescanning promotes the development of a stronger fiber texture aligned with the <100> direction, whereas maintaining the same scanning directions as the initial scan emphasizes the plate texture of (100)<100>. This study highlights the potential of laser rescanning strategies in optimizing the microstructural properties of LPBF-manufactured parts, offering insights into additive manufacturing processes. |

| 10:40am - 11:00am | MAMP3: Incorporating non-linear effects in fast semi-analytical thermal modelling of powder bed fusion | Shaun Cooke, The University of British Columbia  
**Abstract:** The usefulness of semi-analytical thermal models for predicting the connection between process, microstructure and properties in powder bed fusion has been well illustrated in recent years. Such an approach provides the promise of accuracy comparable to tools that are orders of magnitude more computationally expensive. The opportunity to make predictions that span several orders of magnitude in space and time comes at the cost of significant simplifications, limiting fully quantitative predictions without empirical calibration. This approach relies on solving a linear problem meaning that first-order non-linear effects induced by e.g. the temperature dependence of material properties and surface boundary conditions, are not incorporated. Here, we revisit these limitations and highlight ways that temperature varying material properties and radiative heat loss from the melt pool can be systematically accounted for. These corrections, made with an eye to minimizing additional computational overhead, bring the technique’s predictive capability much closer to that of high fidelity thermal simulations. Quantitative comparisons to experiments are used to illustrate the important impact of including such corrections. |

| 11:20am - 11:40am | MAMP4: Printability of a water-atomized low-carbon steel powder by laser powder bed fusion | Mazyar Ansari, Innotech Alberta  
**Abstract:** There has been growing interest in leveraging low-cost water-atomized powder feedstocks for additive manufacturing (AM), which stems from the need to enhance cost-effectiveness and sustainability in AM processes. While water-atomized powder presents numerous advantages and material selection versatility, it is not commonly used as an alternative to gas/plasma-atomized powder. This study focuses on evaluating the printability of water-atomized low-carbon steel (ATOMET1025, RioTinto) in laser powder bed fusion (LPBF). To explore the process window, wide-range and narrow-range parameters of laser power, scanning speed, and hatch spacing were utilized, aiming to... |
optimize these parameters for the highest density and lowest surface roughness. Additionally, we delve into the microstructure and mechanical properties of selected as-printed and heat-treated samples, offering valuable insights into the quality of the printed materials.

11:40am - 12:00pm, May 24
MAMP5: Micro-Spot Laser Direct Energy Deposition of 18Ni Maraging Steel
Christopher Paul, The University of British Columbia, Okanagan (UBCO)
Abstract: Laser direct energy deposition (LDED) machines typically use 1 – 3 mm diameter laser spots to melt feedstock material. This study examines how a 0.3 mm diameter laser affects weld bead characteristics, microstructure, and mechanical properties of commonly used 18Ni maraging steel. A full factorial experiment on printing parameters during single track printing allowed for weld bead shape and size to be characterized. Parameters were selected from these experiments for printing tensile and microstructural samples. Correlation of the welding parameters to the aspect ratio and percent dilution of weld beads showed that powder feed rate had a dominant effect over laser power and scan speed. SEM and energy-dispersive x-ray spectroscopy (EDS/EDX) showed that within the as-built microstructure, titanium and aluminum inclusions exist that are likely a printing defect. Electron back-scatter diffraction allowed for the retained austenite (FCC) and martensite (BCC) phase distribution to be observed throughout the build height of samples. The distribution of FCC and BCC phases was not homogeneous, with the most BCC being present at the middle of the cube and the least being present at the bottom. Simulations of the LDED process mapped the temperature history profile at the three different locations where phase data was gathered. This showed that the location with the lowest amount of FCC had the highest cooling rate; but no direct correlation between build height and phase distribution could be made confidently. The mechanical properties of the material such as Vickers hardness, ultimate tensile strength, yield strength, and strain were all slightly lower than what has been reported previously. Analysis of the microstructure and overall printing process, highlighted that parameters need to be further optimized for mechanical performance and printability. Material behavior with these smaller laser spots is crucial for maximizing the potential of emerging LDED technology.

12:00pm - 12:20pm, May 24
MAMP6: Investigating the wire deposition of TiC-nucleated AA7075 using L-DED and the influence of post-processing heat treatment.
Taha Waqar, University of Waterloo
Abstract: A fundamental issue for additive manufacturing (AM) of AA7075 is its tendency to crack during solidification, due to its relatively large solidification range and the columnar grain structure characteristic of AM processes. In this study, the printability of laser directed energy deposition (L-DED) of AA7075 weld feedstock enhanced with TiC nanoparticles is investigated. It is found that the combination of high laser power along with low travel speed and low wire feed speed results in the reduction of lack of fusion and porosity within the prints. Microstructure analysis shows that the presence of TiC nanoparticles results in grain refinement, with fine equiaxed grains observed within the melt pool leading to the elimination of cracking. The effect of traditional heat treatments in comparison to direct aging is also studied. The microhardness of the build is found to be higher in prints undergoing T6 heat treatments in contrast to directly aged samples.

01:40pm - 02:00pm, May 24
MAMP7: (Invited) Synchrotron Techniques and Their Applications in Additive Manufacturing
Feizhou He, Canadian Light Source
Abstract: Synchrotron light source enabled many advanced techniques for materials characterization. The broadband synchrotron radiation can be used to probe the chemical information and electronic structures of materials. The high intensity of the synchrotron light allows extremely fast measurements, meaning you can follow dynamic processes such as monitoring the phase changes or chemical reactions. Many synchrotron beamlines provide setups for various in-situ experiments. It is safe to say, the researches enabled by synchrotrons are constantly pushing boundaries of materials science and engineering. In this talk, I will introduce a few synchrotron techniques in spectroscopy, imaging and diffraction, and discuss their advantages. I will also showcase a few applications for additive manufacturing materials, such as reconstruction of 3D structure by micro-CT, surface mapping of trace elements, in-situ diffraction on temperature dependence of crystal structures, micro-XRD for grain orientations, etc.

02:00pm - 02:20pm, May 24
MAMP8: Effects of Sc Addition on Rapidly Solidified Al-10Si-0.4Sc (wt. %) Alloy
Akankshya Sahoo, University of Alberta
Abstract: There have been limited efforts to investigate the impact of Sc on hypoeutectic Al-Si alloys. This is mainly due to the challenging presence of brittle eutectic with flaky Si and large brittle AlSc2Si2 (V-phase) precipitates. Rapid solidification (>10^3 K/s) can be used to address the issue of unfavourable eutectic while benefiting from rapid solidification-induced grain refinement, solid solution, and precipitation hardening. This work investigates the effects of minor Sc addition (0.4 wt.%) on Al-10 wt.%Si over a wide range of thermal histories. Using DSC and Impulse Atomization, hypoeutectic Al-10Si-0.4Sc (wt.%), alloys were produced with a wide range of cooling rates (0.1-10^4 K/s). Higher cooling rates of 6700 K/s and above resulted in the modification of eutectic morphologies to become more globular, thus reducing brittleness and mitigating the negative impacts of AlSc2Si2 phase. The Si and AlSc2Si2 phases contributed to the strengthening process in Al-10Si-0.4Sc (wt.%) alloys. On this premise, a solidification continuous cooling transformation (SCCT) diagram was
Abstract Appendix

created, revealing a significant relationship between microstructure/properties that can aid in alloy and process development in additive manufacturing. The AlSc2S2 phase was for the first time revealed as the hardening phase in Al-Si alloys. The Al-10Si-0.4Sc (wt.%) alloys showed a 10% increase in hardness over their non-Sc counterparts.

02:20pm - 02:40pm, May 24
MAMP9: A Closer Examination of the Nature of Atomic Motion in the Interfacial Region of Crystals Upon Approaching Melting
Jiarui Zhang, University of Alberta
Abstract: Copper (Cu) holds a pivotal role in additive manufacturing due to its exceptional thermal and electrical properties, with techniques like Selective Laser Melting (SLM) enabling the layer-by-layer melting of copper powder into three-dimensional parts with intricate geometries and internal structures. It has recently become appreciated that collective motion, which has been evidenced in melting since the early simulations of hard disc melting by Alder and Wainwright, is a ubiquitous and important phenomenon in both the melting process and interfacial dynamics of crystals. We explore this phenomenon further by focusing on the interfacial dynamics of a model crystalline Cu material using molecular dynamics simulations where we emphasize the geometrical nature and spatial extent of the atomic trajectories over the timescale that they are caged, and we also quantify the collective atomic motion on the timescale of the fast beta relaxation time. The determination of the mean square atomic displacement on the fast beta relaxation timescale within the interfacial regions and the crystal interior allows for the precise estimation of the mobile interfacial layer thickness, the mobility gradient in this layer, and the Tammann temperature at which appreciable atomic mobility first arises in crystalline materials. Direct visualization of the atomic trajectories in their cages over the timescale over which the cage persists indicates that they become progressively more anisotropic upon approaching melting point. We also find interstitial point defects to occur in direct association with the stringlets, proving a link between classical defect models of melting and the more recent studies emphasizing the role of collective motion in initiating melting.

02:40pm - 03:00pm, May 24
MAMP10: Continuous Dynamic Recrystallization during Microindentation
Mina Dehghan, University of Calgary
Abstract: Classical continuous dynamic recrystallization (cDRX) is well known to require extreme deformation conditions, such as high strain and strain rates. The occurrence of cDRX follows a sequential step that includes random dislocation development and multiplication, their arrangement into energetically favored elongated cells, the transformation of elongated dislocation cells into elongated subgrains with LAGBs, disintegration of the elongated subgrains into equiaxed subgrains, and finally, the rotation of equiaxed subgrains that causes the transformation of low-angle grain boundaries to high-angle grain boundaries. It is, however, not clear whether the requirement for extreme deformation conditions can be circumvented when these cDRX steps are interrupted in a nonextreme deformation condition, e.g., low strain rates or static deformation; a phenomenon we term interrupted continuous dynamic recrystallization (icDRX). In this study, the icDRX is accomplished by inducing incomplete cDRX steps in a model high stacking fault energy metal (Al) through friction stir processing (FSP), followed by static load microindentation. Using a femtosecond laser ablation combined with the FIB-SEM procedure (LaserFIB) for site-specific liftout and scanning/transmission electron microscopic (S/TEM) to examine the microstructural changes associated with the normal and tangential force components at the specimen’s contact surface during loading, we report fully-developed cDRXed refined grains of approximately 0.7 μm at the apex of the indent. This is attributed to the rotation of FSP-induced cell structures during microindentation, which results in high-angle grain boundaries. Consequently, it can be concluded that prior dislocation cells in metals can be driven to cDRX completion under nonextreme deformation conditions, e.g., low strain rates or static deformation, such as those obtainable during microindentation.

03:20pm - 03:40pm, May 24
MAMP11: Uncovering the Mechanism behind Two-Step Infiltration during Layered Wide Gap Brazing of MAR-M247 using B-containing Filler Metals
Coleton Parks, McMaster University
Abstract: In this study, governing mechanisms occurring during the layered wide-gap brazing process using MAR-M247 and BNI-9 as the high-melt and braze alloys are explored. While numerous studies have previously investigated conventional wide-gap brazing, where the powders are pre-mixed, the layered variant, with the braze alloy powder placed on top of the high-melting powder, has received comparatively little attention. Using Differential Thermal Analysis, Electron and X-ray microscopy, we investigate the origins of a two-stage braze infiltration sequence. To begin with, a series of interrupted brazing treatments were conducted, spanning from initial braze infiltration at 1053°C to complete infiltration at 1150°C. It was found that upon melting at 1053°C, the braze readily infiltrated the MAR-M247 skeleton via capillary action. This initiated stage 1 infiltration, which terminated at 1068°C. Diffusion of B into the MAR-M247 skeleton appeared to result in partial and complete dissolution of fine and coarse MAR-M247 particles. This led to solute accumulation within the melt, raising the braze solidus, halting infiltration. Stage 2 infiltration initiated at 1102°C, with the re-melting of the partially infiltrated braze, which continued until 1150°C, whereby complete infiltration was achieved.

03:40pm - 04:00pm, May 24
MAMP12: Enhancing Mechanical Properties of Al-Cu-Sc Alloy Lattice Structures Through Heat Treatment in Hybrid Investment Casting
Yifan Li, University of Alberta
Abstract: Hybrid Investment Casting (HIC) combines the precision of additive manufacturing with the superior mechanical properties of traditional investment casting. A lattice structure was designed and Al-4.5wt% Cu-0.4wt% Sc alloy was cast using hybrid investment casting approach. The cast alloy was investigated for its microstructure and compressive properties. This study will also address the effect of heat treatment on both microstructure and mechanical properties of Al-4.5wt% Cu-0.4wt% Sc alloy lattice structures fabricated via HIC, including elastic modulus, yield strength and ultimate compressive strength. The findings highlight an enhancement in mechanical properties from heat treatment by changing the microstructure morphology. This presentation aims to demonstrate the role of heat treatment in refining the microstructural features, thereby directly correlating with improvements in mechanical performance of HIC-produced lattice structures and optimizing the manufacturing process of this lattice structure for specific engineering applications.

04:00pm - 04:20pm, May 24
MAMP13: Effect of layer orientation on the dynamic mechanical response of additively manufactured 18%-Ni-M350 maraging steel-high entropy alloy hybrid armour plate
Timothy Odiaka, University of Saskatchewan
Abstract: A hybrid armour plate with layers of 18%-Ni-M350 maraging steel and AlCoCrFeNi high entropy alloy (HEA) has been manufactured using powder-directed energy deposition (p-DED) additive manufacturing (AM) technology. Cylindrical samples (Ø7 mm x 8 mm) with different layer orientations were machined from the hybrid plate in two batches. In one batch, the layers of the hybrid plate were transversely oriented, while in the other batch, the layers were longitudinal oriented. To strengthen the materials, the samples were subjected to heat treatment. The heat treatment cycles included austenitizing at 850 C for 0.5 hours, followed by ageing at 535 C for 0.5 hours. Dynamic impact tests were conducted using an instrumented split Hopkinson pressure bar at impact momentums ranging from 20 to 40 Kg-ms-1. Furthermore, a linear mixed model was fit to statistically analyse the significance of impact pressure and layer orientation on the impact strength and toughness of the hybrid plates. Microstructural examination of the damage evolution in the samples was conducted using optical microscopy and SEM. Electron backscatter diffraction (EBSD) was performed to analyse the texture evolution in the samples during the dynamic impact loading. The impact test results revealed that at lower impact momentums, longitudinally oriented samples had higher impact strength, but lower impact toughness than transversely oriented samples. The longitudinally oriented samples are more susceptible to the formation of adiabatic shear bands (ASB) compared to the transversely oriented samples. Statistical analysis of the experiment showed a significant effect of the interaction between impact pressure and layer orientation on both the impact strength and toughness of the hybrid samples. EBSD analysis indicates that twinning was the key deformation mechanism in the HEA layer of the hybrid samples while slip is more dominant in the maraging steel layer.

04:20pm - 04:40pm, May 24
MAMP14: Direct Energy Deposition and Characterization of NiSi12-wt% Alloy Variants on Inconel 625 Substrate
Mohammad Ibrahim, University of Agder (Grimstad, Norway)
Abstract: To enhance the processability of nickel silicide using direct energy deposition (DED), the present study introduces alloy variations of NiSi12X-wt% deposited onto an Inconel 625 substrate. Titanium, boron, molybdenum, vanadium, and cobalt were strategically incorporated as element X in the NiSi12X-wt% base alloy, and the resulting alloys were deposited as 30 mm tall cylinders onto the substrate. The processability of the various alloys and the resulting characteristics of the prints were analysed using scanning electron microscopy with energy-dispersive X-ray spectroscopy, X-ray diffractometry, optical microscopy, and hardness measurements. Except for the alloys containing additional titanium and boron all samples demonstrate superior results compared to the un-modified NiSi12-wt% base alloy. The vanadium-modified alloy demonstrates excellent properties even in a 50 mm tall test cylinder. The Incone 625 substrate, with a thermal expansion coefficient comparable to nickel silicide, was confirmed as an optimal base for DED prints of NiSi12-wt% alloys.

04:40pm - 05:00pm, May 24
MAMP15: Engineering 3D Nanopatterning via Molecular Beam Holographic Lithography
Tian Tian, University of Alberta
Abstract: Several techniques for direct patterning of nanoscale structures have been developed in the realm of electronics, optics and sensing. Herein, we report a new direct three-dimensional (3D) nanopatterning technique, molecular beam holographic lithography, for the formation of diverse nanostructures based on various materials including metals, oxides and small organic molecules. This technique emulates the interference of coherent laser, but utilizes molecular beam interaction to achieve direct nanopatterning. The nanopatterning process operates in purely dry conditions, eliminating the use of resists and solvents. Patterning of multiple materials to yield binary, ternary up to quaternary 3D nanostructures can be realized using such technique. In addition, we present a computational lithography simulation model to precisely predict the generated patterns and guide the nanopatterning. We anticipate this technique can enable substantial advances in nanopatterning and broaden the applications of versatile nanoscale additive manufacturing.


**Abstract Appendix**

**10:20am - 10:50am, May 23**

CSAE1: (Invited) The Role of Ce Addition on Strain Localization and the Evolution of Portevin-Le Chatelier (PLC) effect in Direct Chill Cast Al-5wt%Mg Alloy

Shengze Yin, Queen's University

Abstract: In this study, Al-5wt%Mg ingots with and without the addition of 1wt%Ce, 0.1wt%Sc, and 0.1wt%Zr were produced through Direct Chill (DC) casting. Tensile tests were performed on the as-cast samples with strain rates ranging from 10-2 to 10-4 mm/mm. Digital Image Correlation (DIC) was used during the tensile tests to help visualize strain localizations. A significant delay in the onset of the Portevin-Le Chatelier (PLC) effect was observed in the Ce-modified sample, extending the deformation range to 9% elongation before serration points emerged. This delay enhances the alloy's formability, a critical factor for the manufacturability of sheet products. When examined under SEM and EDS, in the Ce-added sample, the Al3Mg2 β phase or Al-(Fe,Mn) α phase was found to be replaced by the Ce-rich Al11Ce3 and Al13CeMg6 phases at the cell/grain boundaries. This alteration in the phases formed was further examined using Schien-Gulliver simulations in ThermoCalc Software for Al-5wt%Mg-0.4wt%Fe-0.8wt%Mn with 1wt%Ce addition. For a definitive identification of these secondary phases, higher-resolution EDS and diffraction patterns from TEM are anticipated in forthcoming research. These preliminary results will lay the foundational work and are intended to serve as a baseline for the development of Ce-containing rapidly-solidified Al-5Mg strips using thin strip (TS) casting process.

Therefore, electrochemical hydrogen charging was performed on both AM and CM 316L samples to achieve a comparable hydrogen content in the samples, which were further measured by TDS and GDOES. Identically samples were in-situ / ex-situ charged for tensile test to quantitatively correlate the mechanical degradation by introducing different contents of hydrogen into the sample. A combination of surface characterization techniques; SEM, EBSD, XRD, and EBSD are deployed to accurately characterize and gain an improved understanding of the hydrogen embrittlement mechanism in CM and AM (as-built and heat treated) stainless steel. The higher presence of hydrogen reduced ductility in the as-built AM sample but did not significantly influence the response in CM materials. Hydrogen-charged samples exhibited a large area of brittle fracture mode, while hydrogen-free samples showed ductile fracture morphology.

**11:40am - 12:00pm, May 23**

CSAE4: Stable and Efficient Microbubble-Enhanced Cold Plasma Activation for Treatment of Flowing Water

Ziya Saedi, University of Alberta

Abstract: Cold plasma technology has received immense attention in several fields including wastewater treatment, disinfection, food processing and storage, and agriculture due to its ability to produce reactive species at low energy input. However, the scalability of generation of plasma activated water (PAW) still remains a challenge. Microbubble-enhanced cold plasma activation (MB-CPA) technology leverages small bubbles for effectively interfacing plasma discharge in a gas phase and a flow of liquid media. In this study, we developed a stable and efficient approach for the continuous production of PAW by optimizing the transfer of active species generated during plasma discharge to water flow. Novel Venturi-type microbubble generators were designed for the production of PAW by maximizing the rapid transfer of active species generated during plasma discharge in air. Key geometrical features of the tubes including the position and the opening size of the air inlet were tuned, aiming to transfer active species in a wide range of liquid flow conditions. The performance of our flow systems was evaluated by using pure water, buffered saline, and real river water containing micro-pollutants. We found that MB-CPA can effectively eliminate chemical compounds such as dye and antibiotic residues, as well as biological pathogens like Gram-positive and Gram-negative bacteria. In a cell viability assay, the technology exhibited cytotoxic effects against cancerous cells, specifically HeLa and MCF-07 cell lines. This multifunctionality underscores the versatility of MB-CPA, positioning it as a multifaceted solution for both water and wastewater treatment. Our work shows that the designed MB-CPA system represents a promising and
sustainable technological advancement, offering a green alternative for the widespread activation of water in various applications.

**12:00pm - 12:20pm, May 23**

**CSAE5: Microbubble-Enhanced Cold Plasma for Recycling of Wastewater**  
**Qiuyun Lu, University of Alberta**  
**Abstract:** Cold plasma generated from the high-voltage electrical discharge of gases, is considered as a green technology for chemical-free processes for water treatment, food storage, disinfectant, and sustainable agriculture. The reactive oxygen and nitrogen species (RONSs) contribute to the desirable properties of cold plasma activated water (PAW). However, it remains a great challenge to integrate cold plasma with water treatment in practical applications. The transport of RONS from the discharge in gas phase to water is limited by the gas-liquid interface. Our research team has recently developed a microbubble-enhanced cold plasma activation (MB-CPA) technology for water treatment. A large number of microbubbles generated in a flow of water via a self-suction mechanism by using a Venturi tube. The cloud of bubbles transfer RONS to a continuous water flow. By optimizing the design of Venturi tubes assisted by machine learning, our MB-CPA technology has achieved efficient activation of a large volume of water as demonstrated in a 50-L volume. The activation can fully degradation of model compounds including the mixture of 8 stubborn micropollutants, kill the gram positive and negative bacteria, and hinder the growth of cancer cells. To demonstrate the application of PAW for enhanced growth of plants, water after the MB-CPA treatment is applied in the commercial hydroponic systems. The MB-CPA technology developed in our work may offer a green and sustainable solution for water recycling and move a step forward in water activation on a large scale for boosting plant growth.

**12:20pm - 12:40pm, May 23**

**CSAE6: Exploring phase behavior and control of phase stability in fast pyrolysis oil**  
**Ziting Sun, University of Alberta**  
**Abstract:** Fast pyrolysis oil (FPO), derived from biomass feedstock, has been regarded as a promising carbon-neutral fuel in recent years. However, one of the biggest challenges in the industrial use of FPO is the phase separation that occurs during its storage, transport, and processing. Furthermore, the exact conditions (e.g., chemical composition and temperature) under which this phenomenon occurs have not been thoroughly studied. The objective of this study is to develop a series of ternary phase diagrams to identify the conditions where FPO exhibits kinetic stability. The investigated conditions included the three main components present in FPO (water-soluble content, water-insoluble content, and water). The impact of aging temperature and the doping of a range of organic solvents on the ternary phase diagrams was also studied.

**02:40pm - 03:00pm, May 23**

**CSAE7: On the effect of chemical composition on the Liquid Metal embrittlement susceptibility of advanced high strength steels**  
**Fateme Abdiyan, McMaster University**  
**Abstract:** Because they offer great strength, ductility, and energy absorption at a lower weight, advanced high strength steels are excellent choices for the body in white of automobiles. As a result of this reduced weight, there will be fewer CO2 emissions and less fuel consumed. The issue with these AHSSs is that, although their Zn-coating gives the sheets superior corrosion resistance, it melts during later joining processes like resistance spot welding (RSW), which results in liquid metal embrittlement (LME). LME, which is seen during RSW, is the decrease in elongation to failure of ductile metals. This study aims to assess how various alloying elements, such as Si and Mo, which are crucial for the production of steel, affect the LME susceptibility of steel. The amount of LME cracking in the cross section of samples that have undergone hot tensile testing or welding was measured using an optical microscope. Atom probe tomography revealed the elemental segregation on the grain boundaries at the crack's tip, and electron microscopes were utilized to view the maps of alloying elements in the fractured regions. The results of this investigation demonstrated that while Si weakens the LME response and exacerbates cracking, Mo will strengthen prior austenite grain boundaries to boost resistance to LME.

**03:00pm - 03:20pm, May 23**

**CSAE8: On the Serration Characteristics, Strain Localization Patterns and Crystallographic Texture Development during Tensile Testing of Thermomechanically Processed Thin-Strip Continuous Cast AA5182 Alloy**  
**Hesam Pouraliakbar, Queen’s University**  
**Abstract:** This research investigates how the tensile strain rate affects the Portevin-Le Chatelier (PLC) effect and serration characteristics, and their relationship with the developed crystallographic texture in a rapidly solidified continuously cast thin-strip AA5182 Al-Mg alloy subjected to thermomechanical processing. The newly introduced thin-strip (TS) continuous casting method by Hazelett-CASTechnology(TM) enables the production of 2-5 mm cast aluminum strips with cooling rates approximately two orders of magnitude higher than conventional techniques like direct-chill (DC) casting. This innovative TS casting method streamlines sheet production by eliminating intermediate steps such as scalping, homogenization, and hot rolling, leading to estimated cost savings and higher sustainability by reducing environmental impact. However, the high quench rate inherent in the TS casting process may result in metallurgical properties and responses to post-solidification thermomechanical processes and final mechanical properties differing significantly from those produced by conventional methods, necessitating further investigation. AA5182 alloy samples underwent cold and hot rolling cycles followed by annealing to optimize their formability. Tensile tests at various quasi-static strain rates were conducted.
rates (ranging from 10-4 to 10-1 s-1) were conducted, coupled with digital image correlation (DIC) analysis to examine serration characteristics and strain localization distribution across the tensile gauge. Electron backscatter diffraction (EBSD) scans were performed on both fabricated and tensile samples to analyze crystallographic texture evolution and its correlation with the PLC effect, indicative of dynamic strain aging (DSA). The volume fraction of the primary texture components before and after tensile testing using Euler space, was calculated, and compared while the evolution kinetics and inheritance of components were also investigated.

03:20pm - 03:40pm, May 23
CSAE9: A computationally efficient microstructure evolution model of dynamic recrystallization during hot rolling process
Shabnam Fadaei Chatroudi, McMaster University
Abstract: A novel physically-based mean field model has been developed to describe the microstructural evolution due to recrystallization during deformation. The model has been applied to predict the recrystallized fraction, recrystallized grain size, and flow stress of micro-alloyed steels during discontinuous dynamic recrystallization (DDRX) in hot rolling process. The proposed approach adjusts the simulation grain ensemble in a dynamic manner, ensuring efficiency and accuracy regardless of the number of grains present. This adaptation prevents over-sampling artifacts encountered in case of nucleation of new grains during recrystallization, in addition to explicitly include size distributions in the model. There is a good agreement between model predictions and analytical solutions as well as experimental results obtained in the different recrystallization regimes, opening the possibility of modeling multi-pass operations compatible with industrial applications. The anticipated outcomes of this study would advance our understanding of material behavior in pipeline applications, leading to enhanced safety and reduced adverse environmental consequences resulting from failures. Ultimately, this research endeavors to yield products of higher quality.

04:00pm - 04:20pm, May 23
CSAE10: Modeling of hydrogen atom distribution at corrosion defect on existing pipelines repurposed for hydrogen transport under pressure fluctuations
Jin Zhang, University of Calgary
Abstract: While repurposing the existing pipelines for hydrogen transport contribute to accelerated development of the full-scale hydrogen economy, the suitability of the aged pipelines should be assessed on their hydrogen embrittlement (HE) susceptibility in high-pressure gaseous hydrogen environments. In this work, a three-dimensional mechanics-hydrogen diffusion coupling finite element model was developed to determine the distribution of hydrogen (H) atoms at corrosion defect on pipelines under pressure fluctuations. Parametric effects, including corrosion defect dimensions (i.e., width, length, and depth) and pressure fluctuating parameters (i.e., cyclic load ratio and loading frequency), were determined. A high stress concentration exists in the longitudinal edge of the defect, while the stress level in the circumferential edge is low. The defect center is associated with the greatest stress and stress variation amplitude. H atoms tend to concentrate at the corrosion defect, especially the defect center, representing the most vulnerable site to initiate hydrogen induced cracks. Most H atoms reside at the lattice sites, rather than the traps, indicating a limited capacity of the traps to host H atoms as compared to the crystalline lattice sites. With the increase in defect depth and length, both the stress level and stress variation amplitude at the corrosion defect are apparently elevated. More H atoms accumulate at the defect center, increasing the susceptibility to HE. As a comparison, the HE susceptibility of the corroded pipelines decreases with increased corrosion width. As the cyclic load ratio decreases, less H atoms accumulate at the corrosion defect. A decreasing cyclic loading frequency results in decreased stress variations but an increased H atom concentration at the corrosion center. The results provide a base to control pipeline HE by properly adjusting the operating pressure.

04:20pm - 04:40pm, May 23
CSAE11: Influence of pipeline steel microstructure on hydrogen uptake after gaseous and electrochemical charging
Tonye Jack, University of Saskatchewan
Abstract: With growing global awareness of the urgent need to reduce greenhouse gas emissions, hydrogen has emerged as a pivotal energy carrier for future decarbonization frameworks. To ensure an effective hydrogen economy, this energy carrier needs to be transported over long distances using steel pipelines. To this end, the concerns related to hydrogen embrittlement of these pipelines need to be addressed, and the relationship between microstructure and hydrogen uptake of steel pipes should be determined. Moreover, proper test methods for material qualification and certification must be developed. However, the limited number of test facilities supporting gaseous hydrogen charging and respective mechanical testing poses a significant challenge amid this rising demand. Hence, there is a need for a comparison between the readily available electrochemical testing methods and the scarce gaseous testing methods. This relationship would facilitate the evaluation of pipeline steels for hydrogen transport. Using microstructural analysis, thermal desorption analysis, and hydrogen diffusion studies, the hydrogen uptake after these two ingress mechanisms was compared. Our findings clearly demonstrate that the contribution of various microstructural features to hydrogen uptake and desorption is different. The measurements of hydrogen content revealed that the electrochemical hydrogen ingress is more sensitive to the steel's microstructure than the gaseous hydrogen ingress. Also, dislocation density plays a more important role in facilitating hydrogen gas dissociation, ingress, and retention when compared to the contribution of grain size.
Abstract Appendix

04:40pm - 05:00pm, May 23
CSAE12: Adapting Qatar’s LNG Infrastructure for LH2: Feasibility and Challenges
Sumia Manzoor, Hamad Bin Khalifa University

Abstract: The transition towards sustainable energy sources is essential in addressing the rising global climate concerns. As part of this transition, repurposing existing liquefied natural gas (LNG) infrastructure for the utilization of alternative fuels presents a promising avenue. Qatar is currently one of the leading LNG exporters accounting for a significant portion of global LNG production of 77 million tonnes per annum. Qatar's prominent position as a key player in the LNG market underscores the importance of its role in driving clean energy transitions. Leveraging its expertise and infrastructure in LNG production, storage and distribution, Qatar stands at a critical juncture to spearhead the adoption of alternative fuels such as Liquid Hydrogen (LH2). This study aims to assess technical consideration, such as compatibility, safety and efficiency of the existing liquefaction, storage, and distribution facilities to be utilized for LH2, considering Qatar's unique environmental challenges and goals. Through a comprehensive analysis of the opportunities and challenges associated with repurposing LNG infrastructure for LH2 in Qatar, this research contributes to the broader discourse on advancing clean energy transitions and achieving sustainability goals, while highlighting the pivotal role of Qatar as a leading LNG exporter in shaping the future of energy.
Abstract Appendix

Symposium: Nanomaterials Advancing the Hydrogen Economy (NAHE)
Friday, May 24, 2024
Room: E6-064, ETLC
Chair: Dr. Karthik Shankar

01:40pm - 02:00pm, May 24
NAHE1: (Invited) Role of microstructures in hydrogen diffusion in structural metals
Jun Song, McGill University
Abstract: Hydrogen-microstructure interactions have always been a crucial problem in understanding and predicting hydrogen embrittlement (HE) phenomenon in structural metals. Particularly with respect to hydrogen diffusion, there remain debates on the role of microstructures. For instance, grain boundaries (GBs) and dislocations are often attributed as facilitating hydrogen transport. Yet the experimental and theoretical studies are elusive and even controversial. In this work, hydrogen kinetics at GBs and dislocations in structural metals, Ni and Fe, were systematically investigated to reveal atomic details while enabling long-time (i.e., microsecond to second) hydrogen diffusion analysis. For GBs, we showed that there exists a slow-fast transition in terms of hydrogen diffusion, dependent on the GB characteristics, a transition that can be predicted on the basis of the Frank-Bilby model. For dislocations, they were found to favor hydrogen trapping and provide regions of low migration barriers. However, these regions of low barriers only lead to localized fast short-circuit hydrogen diffusion, but do not translate into fast hydrogen transport over long time, which is attributed to fast hydrogen diffusion pathways along the dislocation line direction being periodically blocked by high hydrogen migration barriers. We further quantitatively analyzed the correlation between hydrogen diffusion behaviors and local dislocation structures, illustrating the structural origin leading to local short-circuit diffusion and inhibition of long-range hydrogen transport at dislocations. The findings provide new knowledge to advance our mechanistic understanding of hydrogen-microstructure interaction in structural metals.

02:00pm - 02:40pm, May 24
Narendra Chaulagain, University of Alberta
Abstract: TiO2 is a n-type, chemically resilient semiconductor capable of functioning as the photoanode in photoelectrochemical (PEC) water splitting to generate H2 and O2. The generated hydrogen is green H2 if sunlight is used as the source of energy incident on the PEC cell or if solar electricity is used to power light emitting diodes (LEDs) that irradiate the PEC cell. The primary disadvantage of using TiO2 in PEC cells is its wide electronic bandgap (3.0-3.2 eV) which renders the photoanode sensitive to high energy ultraviolet photons where only 5% of solar energy resides. Roughly 50% of the energy in sunlight resides in photons with energies of 1-3 eV. Therefore, any techno-economically feasible PEC cell needs to harvest visible photons and a small portion of infrared photons. There is a long scientific history of efforts to sensitize TiO2 with narrow bandgap inorganic semiconductors to increase light harvesting and PEC performance. None of these efforts has been successful due to one or more of three reasons: (i) The bandgap and/or energy levels of the sensitizer are not appropriate for PEC water-splitting (ii) The sensitizer is not photochemically durable and (iii) The kinetics of charge injection and recombination at the TiO2/sensitizer interface are unsuitable. We discuss carbon nitride (CN) sensitizers which are photochemically stable, have moderate-to-low bandgaps, and are capable of injecting photogenerated electrons into TiO2 with low recombination losses. P-doped CN quantum dots with a bandgap of 2.1 eV are excellent sensitizers for anatase phase TiO2 nanotube arrays, generating photocurrent densities of 2.5 mAcm-2 and H2 evolution rates of 22 µmol h−1 in PEC water-splitting under AM1.5G one sun illumination. Low bandgap (Eg = 1.75 eV) carbon-rich CN grown directly on rutile phase TiO2 nanorod arrays, generated a photocurrent density > 4 mAcm-2 and a H2 evolution rate of 27 µmol h−1 in PEC water-splitting when irradiated with AM1.5G simulated sunlight.

02:20pm - 02:40pm, May 24
NAHE3: Environment-friendly Cu:ZnInSe/ZnSeS core/shell QDs sensitized TiO2 photoanode for efficient photoelectrochemical hydrogen production
Kokilavani Shanmugasundaram, Institut National de la Recherche Scientifique
Abstract: Colloidal quantum dots (QDs) are considered building blocks for solar energy devices due to their promising optoelectronic properties, such as size/shape/composition-dependent absorption range covering significant portion of solar spectrum. However, well-performing QDs in solar energy conversion technologies are typically containing toxic heavy metals (e.g., Cd and Pb), which restricts their commercial applications. In this context, eco-friendly Cu-doped ZnInSe QDs emerged as a promising alternative due to their unique merits, including the long lifetime of charge carriers and suitable band structure for charge injection. Nonetheless, the sensitivity of the plain Cu:ZnInSe QDs may induce surface defects that act as charge recombination centers, leading to a severe deterioration of the photoelectrochemical (PEC) performance. Encapsulating a wide band gap material is desirable to mitigate the surface defects/traps for improved optoelectronic properties. Here, we report the synthesis of Cu:ZnInSe/ZnSeS core/composition gradient shell with tuneable shell thickness to understand the influence on optoelectronic properties, consequently PEC performance for hydrogen production. An optimized thick composition gradient shell obtained with low Se/S ratio (n = 2 and r =0.05)
showed broader absorption toward longer wavelength and high PL quantum yield,. Resulting PEC device based on the Cu@ZnInSe/ZnSeS core/shell QDs with n =2 and r = 0.05 exhibited an excellent saturated photocurrent density of 11.7 mA/cm² (at 1 V vs RHE) under one sun illumination (AM 1.5 G, 100 mW/cm²), which is 96% higher than the achieved value of bare Cu@ZnInSe QDs. This works provides insights to design environmental-friendly core/shell QDs based PEC device towards low-cost and efficient hydrogen production.

02:40pm - 03:00pm, May 24
NAHE4: Bismuth oxyhalide based photocatalysts for solar driven green H2 fuel production
Md Masud Rana, University of Alberta
Abstract: We present the synthesis of visible light absorbing layered bismuth oxyiodide (BiOI) photocatalyst and its heterojunctions with few layered graphitic carbon nitrides (g-C3N4). Of late, a family of layered earth-abundant ternary semiconductors namely bismuth oxyhalide (BiOX, X = Cl, Br, I) has drawn attention in photocatalysis research due to internal electric field (IEF) and layered dependent optoelectronic properties. Additionally, these van der Waals layered materials can be exfoliated to their monolayered counter parts to enhance surface area by employing liquid phase exfoliation technique. Within the BiOX family, bismuth oxyiodide (BiOI) is of particular interest due to its narrow bandgap of ~ 1.7 eV and an IEF value of 1.22×1010 Vm-1 in bulk BiOI. However, as a standalone photocatalyst, BiOI experiences a high rate of recombination which limits its photocatalytic performance. A solid solution of BiOBrxI1-x was synthesized to tune the optoelectronic properties. Heterojunctions between BiOI and g-C3N4 demonstrated improved photogenerated charge separation while the BiOBrxI1-x solid solution resulted in tunable band energetics, higher specific surface area and suppression of exciton-phonon interactions. These photocatalysts were tested for solar driven green H2 fuel generation. CNF-Cl was synthesized with programmed annealing while the heterojunction of BiOI/CNF-Cl was prepared using solvothermal method. BiOBrxI1-x solid solution was synthesized by solvothermal technique. Photoelectrochemical water splitting was carried out in an H-cell electrochemical reactor and photocatalytic water splitting was performed in a 30 ml batch reactor under pressurized N2 environment. Under AM1.5G 1 sun illumination, pristine BiOI photoanode produced a H2 evolution rate of 4.35 µmol h-1 while BiOI/CNF-Cl demonstrated a H2 evolution rate of 19.71 µmol h-1. For photocatalysis, BiOX solid solution produced a H2 yield of 17.35 µmol h-1.

03:00pm - 04:00pm, May 24
NAHE6: A combination of first-principle and thermodynamics study of hydrogen uptake on steel
Aliakbar Sheikhzadeh, University of Alberta
Abstract: In recent decades, the cumulative levels of greenhouse gases have contributed to climate change and extreme weather events. Fossil fuels, widely used for energy generation, are a major source of greenhouse gases. In recent years, hydrogen has emerged as a new, zero-emission energy carrier that holds the potential to replace fossil fuels and mitigate greenhouse gas emissions. To optimize costs, either pure or blended hydrogen can be transported through existing natural gas pipelines. However, a notable challenge arises in the form of hydrogen embrittlement (HE) risk, wherein the presence of hydrogen in the pipeline can degrade the mechanical properties of steel. Furthermore, hydrogen transportation in pipelines typically occurs under high-pressure conditions, typically ranging from 5-20 MPa, that alter the HE behavior of the pipeline. This study utilizes density functional theory (DFT) calculations to investigate the influence of the Fe(100) surface on hydrogen uptake. Subsequently, the focus shifts to examining the role of different alloying elements in hydrogen dissociative adsorption, including Ti, Ni, Mo, W, Mn, Co, V, Cr, Al, and Cu. The findings indicate that certain alloys, such as Cu and Al, can prevent hydrogen dissociation, while others like Ti and Ni have the ability to trap atomic hydrogen at the first layer, preventing subsurface diffusion. Following this, a thermodynamic
model is developed to explore the impact of temperature and pressure on hydrogen uptake. Results reveal that operating under high-pressure conditions increases the susceptibility of the surface to hydrogen uptake.

04:00pm - 04:20pm, May 24
NAHE7: Porous and non-porous bimetallic alloy nanoparticle photocatalysts
Harshitha Rajashekhar, University of Alberta
Abstract: Metallic nanoparticles (NPs) are recognized for their exceptional catalytic performance and have found extensive application in fuel cells, hydrogenation processes, catalytic converters in automobiles and the purification of air. Bimetallic alloy NPs are particularly interesting because of their synergetic effect between active sites, usually exhibiting superior optical, electronic, and photocatalytic properties compared to monometallic counterparts. By etching the less noble metal in a bimetallic or trimetallic alloy, sponge-shaped noble metal NPs can be produced with unique capabilities for artificial photosynthesis. Likewise, such bimetallic NPs can either be hosted on an inert support (such as glass) or on a semiconducting support such as TiO2, which in turn, affect the carrier dynamics as studied by femtosecond pump-probe transient absorption spectroscopy. My lab has previously reported on enhanced H2 generation and CO2 photoreduction using anodically formed TiO2 nanotubes loaded with Pt, CuPt, ZnPd and AgCu NPs. In this talk, I will focus on porous and non-porous varieties of AuPt and PdPt bimetallic NPs.

04:20pm - 04:40pm, May 24
NAHE8: p-type carbon nitride for photocatalytic and photoelectrochemical hydrogen generation
Biya Saji, University of Alberta
Abstract: Conventional graphitic carbon nitride (GCN) is a n-type layered Van der Waals semiconducting polymer. GCN has found application as a solution processable, visible light absorbing photocatalyst and photoanode, and is the focus of intense research attention because it combines the thermomechanical resilience and chemical resistance of graphene with a non-zero electronic bandgap. However, the absence of p-type GCN limits its use in the aforementioned applications. Herein we use different strategies organized around boron doping during thermal condensation polymerization, to produce p-type carbon nitride (p-CN) with low-to-moderate electronic bandgap. We also exfoliated the carbon nitride to form two-dimensional nanosheets. GCN and p-CN can be used as electron transport layers (ETLs) and hole transport layers (HTLs) in organic and halide perovskite solar cells, which in turn can be connected to an electrolyzer to generate hydrogen. We examined the use of p-CN as both a photocathode and photoanode in sunlight-driven water-splitting. Additionally, we measured hydrogen generation resulting from the photocatalytic splitting of water by p-CN in the presence of suitable electron- and hole-scavenging sacrificial agents. The hydrogen generation values were compared to those obtained from conventional GCN.

04:40pm - 05:00pm, May 24
NAHE9: 1T&2H-MoS2/Ni3S2 Heterojunction Supported by Nickel Foam for overall Water Splitting
Michael Li, University of Alberta
Abstract: Transition-metal disulfide (TMD) electrocatalysts have emerged as competitive alternatives to noble-metal-based electrocatalysts in the large-scale commercialization of hydrogen production via hydrogen evolution reaction (HER). As a classical TMD, MoS2 coupled with Ni3S2, forming the heterostructure, showed great stability and catalytic performance in alkaline conditions. However, the mechanisms of different phases of MoS2, such as the 1T and 2H phases, coupling with Ni3S2 in bifunctional water splitting are not thoroughly discussed. Herein, this work successfully prepared 1T&2H-MoS2/Ni3S2 heterojunction on the support of nickel foam (NF) through simple hydrothermal methods. In particular, the Raman spectroscopy results show that the evidence of 1T phase MoS2. The metallic nature of 1T-phase MoS2 provides additional active sites and better electrical conductivity, which makes MoS2/Ni3S2 heterojunction exhibit excellent performance and durability in HER. The 1T-MoS2/Ni3S2@NF only requires overpotentials of 91.32, 180.12 and 257.16 mV to achieve current densities of 10, 100 and 500 mA/cm2. In addition, it has also been discovered that the 2H phase of MoS2, which is often seen as an inert phase of molybdate sulfide, shows extraordinary performance in oxygen evolution reaction (OER) when combined with Ni3S2. The 2H-MoS2/Ni3S2@NF takes low overpotentials of 79.71, 329.84 and 359.99 mV for OER at current densities of 10, 200 and 500 mA/cm2. This work not only achieves the successful synthesizing of a cost-effective and excellent transition metal-based electrocatalyst for bifunctional water splitting but also highlights the necessity of studying different phases of MoS2 in the electrocatalytic area.
10:20am - 10:50am, May 23
OMCC1: (Invited) Microstructure Evolution of Amorphous Titanium Oxide: The Role of Environmental Transmission Electron Microscope
Jian Chen, NRC Nano
Abstract: Anatase and rutile are the two main polymorphs in titanium dioxide. Although anatase is less stable than rutile, it has wider applications including catalysis, photocatalysis and dye-sensitized solar cells. In thin film synthesis methods, atomic layer deposition produces films with high conformity, stoichiometric composition, and high density. Employing in-situ transmission electron microscopy (TEM), we investigate the formation process of anatase from amorphous TiO2 (a-TiO2) synthesized by atomic layer deposition (ALD). We find the formation of anatase is dependent on the thickness of a-TiO2. When the thickness of a-TiO2 is less than a specific thickness, titanium sub-oxide of Magnéli phase forms. The kinetic study suggests that the crystallization behavior can be described by Avrami equation while the crystallization behavior of sub-oxide of Magnéli phase is much more complicated.

10:50am - 11:10am, May 23
OMCC2: Operando microwave characterization of carrier dynamics in photodetectors and photocatalysts
Navneet Kumar, University of Alberta
Abstract: High surface area semiconductor nanostructures are beneficial for photocatalysis, bulk heterojunction solar cells and certain types of photosensors but are also subject to carrier trapping and trap-mediated recombination processes. While it is currently highly challenging to obtain situ information regarding recombination and the trapping of both minority and majority carriers in high surface area semiconductor nanostructures under operating conditions, microwave characterization using semiconductor nanostructures integrated on planar microwave resonators offers a potential solution. The scattering parameters (s-parameters) of the microwave resonator are sensitive to variations in the instantaneous complex permittivity of the microwave resonator. We monitored the temporal variation in the resonance frequency and quality factor of different types of metal oxide nanotube arrays placed in the coupling gap of a microwave resonator subjected to illumination by photons of different wavelengths. TiO2, VO2 and SnO2 were among the metal oxides studied. A significant shift in the resonance frequency due to an increase in the capacitance of TNTAs without a corresponding decrease in the quality factor (Q) is indicative of dominant carrier trapping. On the other hand, photogeneration of excess carriers is accompanied by a large decrease in Q. Applying a DC bias (in the dark) on top of the microwave bias that injects majority carriers enables us not change the resonance frequency but decreased the microwave amplitude due to free carrier absorption. Furthermore, the DC voltage level-dependent behavior of the characteristic time constants for the decay of the microwave amplitude following removal of the DC bias was found to be consistent with Poole-Frenkel emission of electrons from the contact across an activation energy barrier.

11:10am - 11:30am, May 23
OMCC3: Axial O ligand modulated Fe-N4 sites for highly efficient electrocatalytic nitrogen reduction
Yang Yang, University of Alberta
Abstract: Electrocatalytic N2 reduction reaction (NRR) presents a sustainable alternative to the Haber-Bosch process for ammonia (NH3) synthesis. Iron phthalocyanine (FePc) has been demonstrated as a promising catalyst for the electrocatalytic NRR. However, FePc with planar symmetric Fe-N4 sites has poor N2 adsorption and activation capabilities, resulting in an unsatisfactory NRR performance. Herein, we develop an axial O coordination strategy to optimize the local electron distribution on FePc for improving N2 adsorption and activation. The as-obtained FePc-O-CP exhibits an excellent NH3 yield rate (59.72 μg h⁻¹ mg⁻¹cat.) and a considerable Faradaic efficiency (13.76%) in 0.1 M HCl. Density functional theory (DFT) calculations verify that the axial O ligand on FePc inhibit the adsorption of H⁺ and enhance the adsorption and activation of N2, thereby greatly promoting NH3 generation. This work reveals the significance of regulating the local coordination environment of single sites for improving electrocatalytic NRR performance and provides a feasible strategy for rational design of atomic-scale active sites.

11:40am - 12:10pm, May 23
OMCC4: (Invited) nanoFAB Centre – A central hub of operando materials characterization
Xuehai Tan, University of Alberta
Abstract: Operando characterizations are critically valuable in many research areas, where understanding the behavior and properties of materials and devices under realistic operating conditions is crucial for gaining insights into reaction mechanisms, degradation processes, and other dynamic phenomena that are difficult or impractical to observe using ex-situ methods. While advanced operando characterization instruments often require significant resources and specialized expertise to acquire and maintain, the nanoFAB, a national open-access training, service, and collaboration center located at the University of Alberta, is devoted to providing a central hub of state-of-the-art operando characterization techniques that are widely accessible and affordable to the scientific community. In this presentation, we highlight some of our operando
Abstract Appendix

characterization capabilities, including in-situ heating/electrochemical TEM, in-situ heating/electrochemical XRD, in-situ electrochemical SAXS, in-situ tensile and compression testing X-Ray Microscopy, and other application examples of in-situ and correlative characterizations.

12:10pm - 12:30pm, May 23
OMCC5: Surface Microlenses for Enhanced Photodegradation of Organic Contaminants in Water
Qiuyun Lu, University of Alberta
Abstract: The global need for clean water requires sustainable technology for purifying contaminated water. Highly efficient solar-driven photodegradation is a sustainable strategy for wastewater treatment. However, solar-driven water treatment suffers from reduced efficiency due to the energy loss in the light treatment, difficulties of facility maintenance, and decentralized and intermittent features of solar irradiation. One promising solution is coupling microlenses (MLs) with solar-driven reactors, optimizing the distribution of solar irradiation in contaminated water for higher photodegradation efficiency of organic contaminants. However, the fabrication of customized MLs for solar-water treatment remains to be developed. In this work, we fabricate MLs and microlens arrays (MLAs) by a solution-based method combined with in-situ photopolymerization, which is highly-tunable and scalable. Both microscopy and optical simulations are applied to characterize the optical properties of different types of MLs. Furthermore, the photodegradation of multiple typical organic pollutants in different water matrices is monitored in the MLs-functionalized reactors under varied irradiation conditions to verify the effectiveness of MLs. The combination of optical simulations and the experimental results helps to further improve the efficiency of solar-driven photodegradation by MLs and assist the design of MLs-functionalized reactors for broader applications.

12:30pm - 12:50pm, May 23
OMCC6: Rare earth Ce-modified V2O5 materials as the cathode for zinc-ion batteries
Xuesong Xie, University of Alberta
Abstract: Since the great strides made in rechargeable zinc batteries based on neutral electrolytes, a growing rise of research has demonstrated its merit as a compelling and transformative energy storage strategy. However, the dissolution of active materials in aqueous electrolytes has consistently presented unavoidable issues over an extended period. Here, we report a pre-doping Ce-modified V2O5 cathode prepared by a one-step hydrothermal synthesis method. The interlayer space can be well-enlarged from 1.1nm to 1.3nm with the doping of the Ce element, without the compromise of electrochemical capacity. Besides the improvement in stability, the Ce-V2O5 cathode delivers superior and predominant cyclic voltammetry (CV) performance at a redox peak of 1.16V/0.9V, whereas the pristine V2O5 shows two typical redox peaks at 1.1V/0.96V and 0.65V/0.5V. In-situ XAS investigation demonstrated that Ce-V2O5 prevents the V-valent from shifting to the negative state during the discharge process. It exhibited a highly reversible oxidation state change for the subsequent charge/discharge cycles and successfully suppressed V dissolution, preventing vanadium-based zinc hydroxide salt precipitation. As a consequence, it achieves 98.53% capacity retention after 1000 cycles at a current density of 1 A g⁻¹. We believe that gaining insight into the mechanism will enhance our understanding of the relationship between capacity fading and the chemical state of the channels for vanadium-based zinc ion batteries.

2:40pm - 3:00pm, May 23
OMCC7: (Invited) In Situ/Operando Studies of Cu Catalysts for Electrochemical CO2 Reduction by Soft X-ray Spectro-microscopic Characterization
Chunyang Zhang, McMaster University
Abstract: Electrochemical carbon dioxide electroreduction (CO2R) is a promising route to generate valuable feedstocks through the conversion of CO2 into hydrocarbon and alcohol products, thereby reducing greenhouse gas emissions and protecting the environment. One of the critical challenges for developing practical CO2R electrocatalysts is determining their structure and chemistry under operating conditions. Such results can then be used to optimize improved, high-performance electrocatalysts. In this work, synchrotron-based scanning transmission X-ray microscopy (STXM) and X-ray spectro-ptychography were used for in situ studies of Cu CO2R electrocatalysts. These methods provided spectroscopic characterization and quantitative oxidation state imaging during sample generation by in situ electrodeposition and under CO2R conditions. The in situ STXM studies of Cu catalysts showed that electrodeposited Cu2O particles were converted to metallic Cu at applied potentials less negative than that for the initiation of CO2R. Under CO2R conditions, both in situ STXM and in situ spectro-ptychography showed metallic Cu is the active catalyst for CO2 reduction. The ~3x better spatial resolution of in situ spectra-ptychography was used to follow morphological changes of a single Cu catalytic particle in the electrochemical regime of CO2R. The results showed that the initial cubic structure of the Cu particle changed to form irregular dendritic-like structures during the CO2R process. In addition, the efforts to achieve operando STXM studies of Cu CO2R catalysts by in situ identifying the CO2R products and qualitatively estimating their amount under operating conditions will be shown and presented.

3:00pm - 3:20pm, May 23
OMCC8: Exploring a New Approach for Porous Bioactive Glass Composites
Marzieh Matinfar, University of Alberta
Abstract: Bioactive glasses (BG) exhibit the unique ability of bone bonding and have been shown to be safe and effective for bone regeneration. However, processing them into 3D porous bone scaffolds remains a challenge. This study presents a novel processing route for fabricating porous bioactive glass (BG) composites. The design
approach builds on our previous proof-of-concept work aimed at creating a formable composite scaffold by mixing 4S55 BG powder and a sodium silicate binder solution, which self-sets in the air. The goal of this study is to optimize the setting time and mechanical properties of the composite bone scaffolds to a range that is practical for clinical applications. A formable composite scaffold is created by blending 4S55 BAG powder with a sodium silicate binder solution, which sets upon acid catalyst addition. The project consists of two main parts: (1) Investigating the binder gelation mechanism, gelation kinetics, and mechanical properties (2) Investigating the BG composite bone scaffolds’ setting time, mechanical properties, and in-vitro degradation. Real-time Raman spectroscopy was utilized to study the chemical structure at the molecular level. Micro-CT and SEM were employed to validate porosity, phase distribution, and microstructure of the scaffolds, pH, binder concentration, type of acid catalyst, and BAG content were adjusted to develop a composite with optimal mechanical properties and setting time for clinical applications.

4:20pm - 4:40pm, May 23
OMCC11: Constructing highly dispersed nickel atoms in bamboo like-carbon nanotubes for efficient oxygen reduction
Yifan Li, University of Alberta
Abstract: Single-atom catalysts have been extensively studied for the development of efficient oxygen reduction electrocatalysts due to their high atom utilization and coordinately unsaturated active sites. Carbon nanotubes, as a typical one-dimensional carbon structure, offer enhanced support for loading metal atoms, which can significantly improve the activity and stability of the oxygen reduction electrocatalysts. Up to now, various strategies have been reported to synthesize single atom catalysts with carbon nanotube support, such as impregnation, electrochemical deposition, and defect engineering strategy. However, they often result in inferior oxygen reduction reaction performance due to the low metal atom loading and the weak interactions between metal and the supports. Herein, we reported a bamboo-like one-dimensional carbon nanostructure with highly dispersed Ni single atoms derived from zeolitic imidazolate frameworks (ZIFs). During the pyrolysis process, Ni complexes were used to induce the transformation of ZIF-8 with dispersed Ni atoms from a regular dodecahedron structure to a bamboo-like carbon nanotube structure. Benefiting from the excellent electron transport in the bamboo-like carbon structure and the strong electronic coupling between Ni atoms and the N-doped carbon support, this catalyst exhibits excellent oxygen reduction reaction performance comparable to commercial Pt/C catalysts in alkaline solution.

4:40pm - 5:00pm, May 23
OMCC12: Lightweight Al3Ti-based medium-entropy alloys with well-balanced strength and ductility at room and elevated temperatures
Guijiang Diao, University of Alberta
Abstract: One of advantages of multi-element high-entropy or medium-entropy alloys (HEAs/MEAs) is their flexibility for microstructure manipulation, which greatly facilitates obtaining optimal combinations of high

3:20pm - 3:40pm, May 23
OMCC9: The Nanoindentation Response of Single Crystal Magnesium Using a Finite Element Model That Incorporates the Slip Systems
Syed Taha Khursheed, University of Manitoba
Abstract: Nanoindentation is a testing technique used to measure the mechanical properties of materials at very small scales, typically at the nanoscale. It involves using a sharp indenter to apply a precisely controlled force or displacement to the surface of a material and measuring the resulting deformation or penetration depth. While complex stress states and varying elastic-plastic deformation occur beneath the indenter, it is essential to simulate the experiment using a finite element software as it divides up the sample into numerous elements and computes the stress states region wise ensuring the possibility of elastic and plastic regions to occur concurrently. However, the conventional FEM software uses material models that are based on the bulk material properties and increases the inaccuracy of the simulated result. To counter this, a user material subroutine was developed for the first time on the ANSYS Parametric Design Language (APDL) platform that considers the crystal anisotropy, both elastically and plastically, and the crystal plasticity constitutive laws of the Hexagonal Closed Packed structure of Magnesium. This material model is then paired with the contact and loading conditions during the nano-indentation test to obtain the complex state of stress in each element and the load displacement graph. The simulation results will be validated by the nano-indentation test results that are to be obtained from the individual Mg grains.

4:00pm - 4:20pm, May 23
OMCC10: (Invited) Synchrotron Techniques and Their Applications in Additive Manufacturing
Feizhou He, Canadian Light Sources
Abstract: Synchrotron light source enabled many advanced techniques for materials characterization. The broadband synchrotron radiation can be used to probe the chemical information and electronic structures of materials. The high intensity of the synchrotron light allows extremely fast measurements, meaning you can follow dynamic processes such as monitoring the phase changes or chemical reactions. Many synchrotron beamlines provide setups for various in-situ experiments. It is safe to say, the researches enabled by synchrotrons are constantly pushing boundaries of materials science and engineering. In this talk, I will introduce a few synchrotron techniques in spectroscopy, imaging and diffraction, and discuss their advantages. I will also showcase a few applications for additive manufacturing materials, such as reconstruction of 3D structure by micro-CT, surface mapping of trace elements, in-situ diffraction on temperature dependence of crystal structures, micro-XRD for grain orientations, etc.
strength and high ductility in good balance. Based on this phenomenon, we changed Al3Ti intermetallics by introducing additional elements, such as Cr, Mn, Fe and Cu, to an Al3Ti-based lightweight MEA for enlarged room-temperature ductility and improved strength-ductility combination at both room and elevated temperatures. With such modification, the host structure of Al3Ti was changed from brittle D022 to ductile L12 one. Ti and Fe promoted the formation of hard B2 phase, while Cr and Mn favored the formation of D8a phase, which strengthened the alloy at the minor expense of ductility. The compressive yield strength, maximum strength and fracture strain of the lightweight MEA, Al60Ti20Cr5Mn5Fe5Cu5 with a density of 3.88 g/cm3, at room temperature are 520 MPa, 1250 MPa, and 18%, respectively. While the properties changed to 440 MPa, 960 MPa and 24% at 500°C, respectively. The information obtained from this study provides useful information for guiding design Al3Ti-based lightweight MEAs with desirable properties.

5:00pm - 5:20pm, May 23
OMCC13: (Virtual) Advanced Characterization of Nanostructured Energy Materials
Babak Shalchi, NRCan CanmetMATERIALS
Abstract: This talk presents CanmetMATERIALS contribution to the field of energy materials including advanced characterization of nanostructured materials for energy storage, emphasizing the development and analysis of materials for hydrogen storage, lithium-ion batteries (LiBs), supercapacitors, and solid-oxide fuel cells (SOFCs). These works involve multilayered nanostructures with destabilized magnesium hydrides for hydrogen storage, silicon-based anodes for LiBs, core-shell nanostructures for fuel cells, recycled graphite from black mass for LiB anodes, and cobalt-free, tungsten-doped cathodes for LiBs. Central to our approach is the use of transmission electron microscopy (TEM) to explore the relationship between microstructure and properties of these materials. This technique has been instrumental in identifying key microstructural features that influence the materials’ performance. Our research contributes to the understanding of material behavior at the nanoscale, guiding the design of energy storage materials with improved efficiency and sustainability. By examining microstructure-property correlations, we aim to enhance the functionality and environmental compatibility of energy storage systems.