

Technical Meeting and Exhibition

# MS&T21

MATERIALS SCIENCE & TECHNOLOGY

In-Person Event: OCTOBER 17-20, 2021 • COLUMBUS, OHIO

On-Demand Content available: OCTOBER 22-DECEMBER 31, 2021

## TECHNICAL PROGRAM

The content in the technical program was generated on October 11, 2021. Please refer to the online session sheets for the most up-to-date information.



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# Program At A Glance

Information as of October 11. Individual talks are listed on session room signs and the MS&T mobile app.

There will be two ways to access this year's technical programming content: at the in-person MS&T conference in Columbus, Ohio, October 17-20, or as on-demand presentations, which can be viewed remotely October 22 through December 31, 2021.

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ACerS Frontiers of Science and Society - Rustum Roy Lecture	TUE	PM	B130	38
ACerS GOMD Alfred R. Cooper Award Session	TUE	PM	B231	44
Acers Navrotsky Award for Experimental Thermodynamics of Solids	MON	AM	A221	24
ACerS/EPDC: Arthur L. Friedberg Ceramic Engineering Tutorial and Lecture	MON	AM	B130	11
<b>Additive Manufacturing</b>				
<b>Additive Manufacturing: Advanced Characterization for Industrial Applications</b>				
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<b>Additive Manufacturing: Alloy Design to Develop New Feedstock Materials III</b>				
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<b>Additive Manufacturing: Large-Scale Metal Additive Manufacturing</b>				
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Topic Area/Symposium	Date	Time	Room	Page
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Topic Area/Symposium	Date	Time	Room	Page
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Modeling	TUE	PM	EH B	77

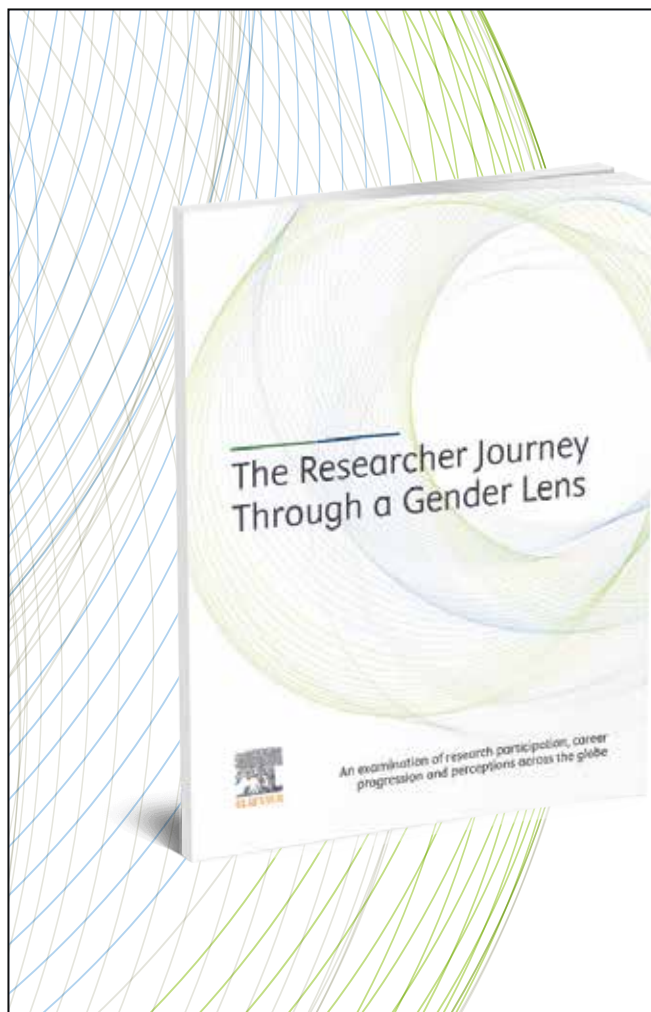


# Program At A Glance

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13th International Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing				
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Processing and Product Manufacturing	TUE	PM	EH B	75

Topic Area/Symposium	Date	Time	Room	Page
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Input to the National Strategic Plan for Advanced Manufacturing	TUE	PM	B130	46
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**Key:** USB = Union Station Ballroom, OND = On Demand, EH = Exhibit Hall



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## PROCESSING AND MANUFACTURING

### 13th Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing — Sustainable Manufacturing of Ceramics

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Surojit Gupta, University of North Dakota; Rajiv Asthana, University of Wisconsin; Hisayuki Suematsu, Nagaoka University of Technology; Mritunjay Singh, Ohio Aerospace Institute; Enrico Bernardo, University of Padova; Yiquan Wu, Alfred University; Zhengyi Fu, Wuhan University of Technology; Allen Apblett, Oklahoma State University; Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology

**Monday AM | October 18, 2021**  
**A212 | Greater Columbus Convention Center**

**Session Chairs:** Allen Apblett, Oklahoma State University; Luca Masi, Ansys Inc.

**8:00 AM**

**The Use of Waste Materials for the Manufacture of Ceramic Water Filters in Marginalized Communities:** *Ian Nettleship*<sup>1</sup>; Chuyuan Zheng<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**8:20 AM Invited**

**Single Source Precursors for Lanthanum Phosphates:** *Allen Apblett*<sup>1</sup>; Mha Albqmi<sup>1</sup>; <sup>1</sup>Oklahoma State University

**8:50 AM**

**Bandgap Engineering of Epitaxial  $\alpha$ -(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> Films Grown via the Spin-coating Method:** *Iva Milisavljevic*<sup>1</sup>; Yiquan Wu<sup>1</sup>; <sup>1</sup>Alfred University

**9:10 AM**

**Development of Energy Efficient Solid-state Material Processing Technologies for Sustainable Manufacturing:** *Kumar Kandasamy*<sup>1</sup>; <sup>1</sup>Enabled Engineering

**9:30 AM**

**Green Method for Preparation of Inorganic Green Pigments:** *Allen Apblett*<sup>1</sup>; Travis Reed<sup>1</sup>; <sup>1</sup>Oklahoma State University

## ARTIFICIAL INTELLIGENCE

### Accelerating Materials Science with Big Data and Machine Learning — Session I

**Program Organizers:** Huan Tran, Georgia Institute of Technology; Muratahan Aykol, Toyota Research Institute

**Monday AM | October 18, 2021**  
**A123 | Greater Columbus Convention Center**

**Session Chair:** Huan Tran, Georgia Institute of Technology

**8:00 AM Invited**

**Considerations for Interpretability, Reliability, And Data-efficiency in Machine Learning Properties of Solid-state Materials:** *Christopher Sutton*<sup>1</sup>; <sup>1</sup>University of South Carolina

**8:40 AM Invited**

**Searching for New Ferroelectric Materials Browsing a High-throughput Phonon Database:** Maksim Markov<sup>1</sup>; Louis Alaerts<sup>2</sup>; Henrique Miranda<sup>1</sup>; Guido Petretto<sup>1</sup>; Wei Chen<sup>1</sup>; Janine George<sup>1</sup>; Eric Bousquet<sup>3</sup>; Philippe Ghosez<sup>3</sup>; Gian-Marco Rignanese<sup>1</sup>; *Geoffroy Hautier*<sup>4</sup>; <sup>1</sup>UCLouvain; <sup>2</sup>Dartmouth College; <sup>3</sup>Université de Liège; <sup>4</sup>Dartmouth

**9:20 AM**

**Slip Band Characterization with Microtensile Testing Using Digital Image Processing:** *Anthony Lombardi*<sup>1</sup>; Elim Schenck<sup>1</sup>; Subhasish Malik<sup>1</sup>; Ajit Achuthan<sup>1</sup>; Sean Banerjee<sup>1</sup>; Natasha Banerjee<sup>1</sup>; <sup>1</sup>Clarkson University

**9:40 AM**

**Materials Graph Ontology for Improving the Standardization and Utilization of Materials Data:** *Sven Voigt*<sup>1</sup>; Surya Kalidindi<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

## SPECIAL TOPICS

### ACerS Education and Professional Development Symposium — Introduction to Education and Professional Development Opportunities

**Sponsored by:** ACerS Education and Professional Development Council

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Yolanda Natividad, American Ceramic Society; Ashley Hilmas, Air Force Research Laboratory

**Monday AM | October 18, 2021**  
**B142/143 | Greater Columbus Convention Center**

**Session Chairs:** Jessica Rimsza, Sandia National Laboratories; Ashley Hilmas, Air Force Research Laboratory

**8:00 AM**

**Grad School: An Entrée into the Knowledge Creation Enterprise:** *Frank Zok*<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

**8:30 AM**

**Individual Benefits of Diversity in the Workplace:** *Ryan McCarty*<sup>1</sup>; Victoria Christensen<sup>2</sup>; <sup>1</sup>University of California Irvine; <sup>2</sup>University of California Santa Barbara

**9:00 AM**

**The Materialism Podcast: A New Medium for Materials Science Education:** *Taylor Sparks*<sup>1</sup>; Andrew Falkowski<sup>1</sup>; <sup>1</sup>University of Utah

**9:30 AM**

**Professional Development Opportunities with The American Ceramic Society:** *Mark Mecklenborg*<sup>1</sup>; <sup>1</sup>The American Ceramic Society

**10:00 AM Break**

**10:20 AM**

**Real Innovation in the 21st Century – How Can Business Do It?:** *Cullen Hackler*<sup>1</sup>; <sup>1</sup>PEI

**10:50 AM** Panel Discussion Experiences with EPDC and ACerS



# Technical Program

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## SPECIAL TOPICS

### ACerS/EPDC: Arthur L. Friedberg Ceramic Engineering Tutorial and Lecture

*Sponsored by:* ACerS/Education and Professional Development Council

**Monday AM | October 18, 2021**  
**B130 | Greater Columbus Convention Center**

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**9:00 AM Invited**

**Environmental Barrier Coatings – Enabling Materials for Extreme Environments:** *Elizabeth Opila*<sup>1</sup>; <sup>1</sup>University of Virginia

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## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — AM Modeling - Microstructures & Defects

*Sponsored by:* TMS Computational Materials Science and Engineering Committee

*Program Organizers:* Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

**Monday AM | October 18, 2021**  
**A113 | Greater Columbus Convention Center**

*Session Chairs:* Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, CCDC Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeon-Gil Jung, Changwon National University

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**8:00 AM**

**Spattering and Associated Pore Formation Modeling for Laser Powder Bed Fusion of Inconel 718:** *Qian Chen*<sup>1</sup>; chaitanya Vallabh<sup>1</sup>; Albert To<sup>1</sup>; Xiayun Zhao<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**8:20 AM**

**Mitigating Stray Grain Nucleation during the Laser Powder Bed Fusion of Single Crystal CMSX-4:** *Runbo Jiang*<sup>1</sup>; Zhongshu Ren<sup>2</sup>; Tao Sun<sup>2</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>University of Virginia

**8:40 AM**

**Cellular Automaton Simulation of Three-dimensional Microstructure Evolution during Powder Bed Fusion Additive Manufacturing:** *Michael Moodispaw*<sup>1</sup>; Cheng Gu<sup>1</sup>; Alan Luo<sup>1</sup>; Qigui Wang<sup>2</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>General Motors

**9:00 AM**

**A Computational Approach for Establishing Microstructure-property Relationships for Additively Manufactured IN718:** *An Nguyen*<sup>1</sup>; Jason Mayeur<sup>1</sup>; <sup>1</sup>The University of Alabama in Huntsville

**9:20 AM**

**A Microstructure-informed Multiscale Computational Model for Additively Manufactured (AM) Metals and Alloys:** *Chamara Herath*<sup>1</sup>; Ajit Achuthan<sup>1</sup>; <sup>1</sup>Clarkson University

**9:40 AM**

**Multiscale Material Modeling of Laser Powder Bed Fusion Additive Manufacturing Soft Magnetic Composites:** *Li Ma*<sup>1</sup>; Caleb Andrew<sup>2</sup>; Ryan Carter<sup>1</sup>; Ian McCue<sup>1</sup>; Joe Sopcisak<sup>1</sup>; Mitra Taheri<sup>2</sup>; <sup>1</sup>Johns Hopkins University Applied Physics Laboratory; <sup>2</sup>Johns Hopkins University

**10:20 AM Break**

**10:40 AM**

**CFD Simulations for Additive Manufacturing:** *Pareekshith Allu*<sup>1</sup>; <sup>1</sup>Flow Science Inc.

**11:00 AM**

**Comparison of Commercial Additive Manufacturing Simulation Tools for Full Build Analysis:** *Adam Gershen*<sup>1</sup>; Charles Fisher<sup>1</sup>; <sup>1</sup>Naval Surface Warfare Center, Carderock Division

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Ceramic-based Materials: Process Development, Materials, Process Optimization and Applications — Session I: Extrusion-based AM

*Sponsored by:* ACerS Engineering Ceramics Division, ACerS Basic Science Division, ACerS Manufacturing Division

*Program Organizers:* Xuan Song, University of Iowa; Lei Chen, University of Michigan-Dearborn; Xiangyang Dong, Missouri University of Science and Technology; Yiquan Wu, Alfred University; Paolo Colombo, University of Padova; Rajendra Bordia, Clemson University; Long-Qing Chen, Pennsylvania State University

**Monday AM | October 18, 2021**  
**A112 | Greater Columbus Convention Center**

*Session Chairs:* Rajendra Bordia, Clemson University; Xuan Song, University of Iowa

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**8:00 AM Invited**

**A Review of Extrusion-based AM via Robocasting:** *Joe Cesarano*<sup>1</sup>; <sup>1</sup>Robocasting Enterprises

**8:30 AM**

**Extrusion-based Additive Manufacturing of Silicon Carbide:** *Ruoyu Chen*<sup>1</sup>; Adam Bratten<sup>1</sup>; *Joshua Rittenhouse*<sup>1</sup>; Haiming Wen<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

**8:50 AM**

**Highly Loaded Aqueous Silicon Carbide Suspensions for Direct Ink Writing:** *Tess Marconie*<sup>1</sup>; Kyle Cox<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; Rodney Trice<sup>1</sup>; <sup>1</sup>Purdue University

**9:10 AM**

**The Influence of Print Layer Orientation on Silicon Carbide Formed via Direct Ink Writing:** *Kyle Cox*<sup>1</sup>; Tess Marconie<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; Rodney Trice<sup>1</sup>; <sup>1</sup>Purdue University

**9:30 AM**

**Examining the Changes in Micro-mechanical Properties of 3D Printed Cement Paste Using Grid Nanoindentation Coupled with SEM/EDS:** Michael Kossow<sup>1</sup>; Lesa Brown<sup>1</sup>; Florence Sanchez<sup>1</sup>; <sup>1</sup>Vanderbilt University

**9:50 AM Invited**

**Additive Manufacturing of Ceramics for Aerospace Applications:** Lisa Rueschhoff<sup>1</sup>; William Costakis<sup>1</sup>; Connor Wyckoff<sup>1</sup>; Matthew Dickerson<sup>1</sup>; Michael Cinibulk<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory

**10:20 AM Break**

**10:40 AM**

**Out of the Lab: 3D Printing on Non-ideal Surfaces:** Domenic Cipollone<sup>1</sup>; Javier Mena<sup>1</sup>; Konstantinos Sierros<sup>1</sup>; Edward Sabolsky<sup>1</sup>; <sup>1</sup>West Virginia University

## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Al-based Alloys

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

**Monday AM | October 18, 2021**

**A115 | Greater Columbus Convention Center**

**Session Chair:** Jovid Rakhmonov, Northwestern University

**8:00 AM**

**Additively Manufactured AlSi10Mg Thin Fins via Laser Powder Bed Fusion: A Parametric Analysis:** Adnen Mezghani<sup>1</sup>; Abdalla Nassar<sup>2</sup>; Timothy Simpson<sup>1</sup>; <sup>1</sup>Pennsylvania State University; <sup>2</sup>Applied Research Laboratory

**8:20 AM**

**Effect of Direct Metal Laser Sintering Build Parameters on Defects and Ultrasonic Fatigue Performance of Additively Manufactured AlSi10Mg:** Robert Rhein<sup>1</sup>; Qianying Shi<sup>2</sup>; Srinivasan Arjun Tekalur<sup>1</sup>; J Wayne Jones<sup>2</sup>; Jason Carroll<sup>1</sup>; <sup>1</sup>Eaton Corporation; <sup>2</sup>University of Michigan

**8:40 AM**

**Effects of Process Parameters, Post-processing, and Defects on Tension and Fatigue Properties of LPBF AlSi10Mg:** Austin Ngo<sup>1</sup>; Collin Sharpe<sup>1</sup>; Varthula Jayasekera<sup>2</sup>; Brett Conner<sup>2</sup>; Holly Martin<sup>2</sup>; Christopher Tuma<sup>1</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>Youngstown State University

**9:00 AM**

**Effects of Process Parameters and Defects on S-N Fatigue of LPBF AlSi10Mg:** Collin Sharpe<sup>1</sup>; Austin Ngo<sup>1</sup>; Christopher Tuma<sup>1</sup>; Michael Shinohara<sup>1</sup>; Holly Martin<sup>2</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>Youngstown State University

**9:20 AM**

**Process Optimization and Microstructural Analysis for Laser Powder Bed Fusion of AlMgZr Alloy:** Nellie Pestian<sup>1</sup>; Thomas Carmody<sup>1</sup>; Daniel Satko<sup>1</sup>; Evan Diewald<sup>2</sup>; Christian Gobert<sup>2</sup>; Anthony Rollett<sup>2</sup>; Jack Beuth<sup>2</sup>; Ayman Salem<sup>1</sup>; Nam Phan<sup>3</sup>; Jan Kasprzak<sup>3</sup>; <sup>1</sup>MRL Materials Resources LLC; <sup>2</sup>Carnegie Mellon University; <sup>3</sup>Naval Air Systems Command

**9:40 AM**

**Characterization of Near-eutectic Al-Ce with Sc and Zr Microadditions Processed by Rapid Laser Remelting:** Jovid Rakhmonov<sup>1</sup>; Clement Ekaputra<sup>1</sup>; David Weiss<sup>2</sup>; David Dunand<sup>1</sup>; <sup>1</sup>Northwestern University; <sup>2</sup>Eck Industries, Inc.

## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: ICME Gaps: Material Property and Validation Data to Support Certification — Data Needs for Simulation: Material Property and Validation Data to Support Certification

**Sponsored by:** TMS: Integrated Computational Materials Engineering Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Joshua Fody, NASA Langley Research Center; Edward Glaessgen, NASA Langley Research Center; Christopher Lang, NASA Langley Research Center; Greta Lindwall, KTH Royal Institute of Technology; Michael Sansoucie, NASA Marshall Space Flight Center; Mark Stoudt, National Institute of Standards and Technology

**Monday AM | October 18, 2021**

**A114 | Greater Columbus Convention Center**

**Session Chairs:** Christopher Lang, NASA Langley Research Center; Joshua Fody, NASA

**8:00 AM Introductory Comments**

**8:10 AM Keynote**

**ICME Gaps for Additive Manufacturing of Metals:** Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**8:50 AM**

**High Temperature Material Property Data and Challenges to Thermal Process Model Predictions and In-Situ/Ex-Situ Measurements for Metallic Additive Manufacturing:** Joshua Fody<sup>1</sup>; Samuel Hocker<sup>1</sup>; Joseph Zalameda<sup>1</sup>; Wesley Tayon<sup>1</sup>; <sup>1</sup>NASA Langley Research Center

**9:10 AM**

**Determining Data Requirements to Quantify Porosity in the Laser Powder Bed Fusion Process:** Mahya Shahabi<sup>1</sup>; Caitlin Kean<sup>1</sup>; Adrianna Yuen<sup>1</sup>; Anthony Rollett<sup>2</sup>; Sneha Prabha Narra<sup>2</sup>; <sup>1</sup>Worcester Polytechnic Institute; <sup>2</sup>Carnegie Mellon University

**9:30 AM**

**Methods for Improved Part-scale Thermal Process Simulations in Laser Powder Bed Fusion:** Seth Strayer<sup>1</sup>; Florian Dugast<sup>1</sup>; Alaaeldin Olleak<sup>1</sup>; Shawn Hinnebusch<sup>1</sup>; Joshua Fody<sup>2</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>National Aeronautics and Space Administration

**9:50 AM**

**Experimental and Numerical Investigation of Pressureless Sintering for Binder Jetted Metal Parts:** Kaiwen Zhang<sup>1</sup>; Wei Zhang<sup>1</sup>; Ryan Brune<sup>1</sup>; Xu Zhang<sup>1</sup>; Edward Herderick<sup>1</sup>; <sup>1</sup>Ohio State University

# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Advanced Characterization for Industrial Applications — In-situ and Operando Techniques

**Sponsored by:** TMS Advanced Characterization, Testing, and Simulation Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Nadia Kouraytem, Utah State University; Fan Zhang, National Institute of Standards and Technology; Lianyi Chen, University of Wisconsin-Madison

**Monday AM | October 18, 2021**  
**A121 | Greater Columbus Convention Center**

**Session Chair:** Nadia Kouraytem, Utah State University

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**8:00 AM** Introductory Comments

**8:10 AM**

**Characterizing Powder Spreading Dynamics in Powder Bed Fusion AM Process by High-speed X-ray Imaging:** *Luis Escano*<sup>1</sup>; Lianyi Chen<sup>1</sup>; <sup>1</sup>University of Wisconsin - Madison

**8:30 AM**

**Domain Adaption for Enhanced X-ray CT Reconstruction of Metal Additively Manufactured Parts:** *Amir Ziajari*<sup>1</sup>; Abhishek Dubey<sup>2</sup>; Singanallur Venkatakrishnan<sup>1</sup>; Michael Sprayberry<sup>1</sup>; Curtis Frederick<sup>3</sup>; Paul Brackman<sup>3</sup>; Philip Bingham<sup>1</sup>; Ryan Dehoff<sup>1</sup>; Vincent Paquit<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>NIH; <sup>3</sup>Carl Zeiss Industrial Metrology, LLC

**8:50 AM**

**In-situ Quality Monitoring of PBF AM Parts:** *Bernard Revaz*<sup>1</sup>; <sup>1</sup>SENSIMA Inspection/AMQuam SA

**9:10 AM**

**Understanding the Keyhole Dynamics in Laser Welding Using Time-resolved X-ray Imaging Coupled with Computer Vision and Data Analytics:** *Joseph Aroh*<sup>1</sup>; Jongchan Pyeon<sup>1</sup>; Runbo Jiang<sup>1</sup>; Benjamin Gould<sup>2</sup>; Andy Ramlatchan<sup>3</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Argonne National Laboratory; <sup>3</sup>NASA Langley Research Center

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Alloy Design to Develop New Feedstock Materials III — Modeling and Experiments

**Sponsored by:** TMS Alloy Phases Committee

**Program Organizers:** Aurelien Perron, Lawrence Livermore National Laboratory; Joseph McKeown, Lawrence Livermore National Laboratory; Manyalibo Matthews, Lawrence Livermore National Laboratory; Peter Hosemann, University of California, Berkeley; Christian Leinenbach, Empa, Swiss Federal Laboratories for Materials Science and Technology

**Monday AM | October 18, 2021**  
**A111 | Greater Columbus Convention Center**

**Session Chair:** Aurelien Perron, Lawrence Livermore National Laboratory

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**10:00 AM**

**Insights into Additive Manufacturability and Microstructure Evolution from Simple Analytical Models:** *Charles Smith*<sup>1</sup>; Madeleine Johnson<sup>1</sup>; Olivia DeNonno<sup>1</sup>; Luc Hagen<sup>1</sup>; Daniel Gifford<sup>1</sup>; Juan Gonzalez<sup>1</sup>; Anthony Petrella<sup>1</sup>; Zhenzhen Yu<sup>1</sup>; Amy Clarke<sup>1</sup>; Jonah Klemm-Toole<sup>1</sup>; <sup>1</sup>Colorado School of Mines

**10:20 AM** Invited

**A High-throughput Method to Define New Feedstock Process Parameters in Additive Manufacturing:** *Zahabul Islam*<sup>1</sup>; Ankur Agrawal<sup>1</sup>; Behzad Rankouhi<sup>1</sup>; Frank Pfefferkorn<sup>1</sup>; Dan Thoma<sup>1</sup>; <sup>1</sup>University of Wisconsin

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — Session I

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**Monday AM | October 18, 2021**  
**A120 | Greater Columbus Convention Center**

**Session Chair:** Ola Harrysson, North Carolina State University

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**8:00 AM**

**A Machine Learning Model to Predict Tensile Properties of Ti6Al4V Parts Prepared by Selective Laser Melting with Hot Isostatic Pressing:** *Zhaotong Yang*<sup>1</sup>; Mei Yang<sup>1</sup>; Richard Sisson<sup>1</sup>; Yanhua Li<sup>1</sup>; Jianyu Liang<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**8:20 AM**

**An Infill Strategy for Eliminating Local Hot Spots in Ti64 Laser Powder Bed Fusion:** Evan Diewald<sup>1</sup>; Christian Gobert<sup>1</sup>; *Jack Beuth*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**8:40 AM**

**Effect of Powder Feedstock Size on the Characteristics of Ti6Al4V Lightweight Features from Laser Powder Bed Fusion Additive Manufacturing: An Experimental Study:** Sayed Saghaian<sup>1</sup>; Jonah Hermes<sup>1</sup>; Li Yang<sup>1</sup>; <sup>1</sup>University of Louisville

**9:00 AM Invited**

**Processing to Microstructure to Properties in Titanium:** Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**9:40 AM**

**Effects of Process Parameters on Fatigue Behavior and Defect Characteristics in LPBF Ti-6Al-4V:** Austin Ngo<sup>1</sup>; David Scannapieco<sup>1</sup>; Hunter Taylor<sup>2</sup>; Ryan Wicker<sup>2</sup>; Joseph Pauza<sup>3</sup>; Anthony Rollett<sup>3</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>University of Texas at El Paso; <sup>3</sup>Carnegie Mellon University

**10:00 AM Break**

**10:20 AM**

**Fatigue Fracture Surface Defect Quantification for LPBF Additively Manufactured Ti-6Al-4V:** David Scannapieco<sup>1</sup>; Austin Ngo<sup>1</sup>; Collin Sharpe<sup>1</sup>; Hunter Taylor<sup>1</sup>; Ryan Wicker<sup>1</sup>; Joseph Pauza<sup>1</sup>; Anthony Rollett<sup>1</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University

**10:40 AM**

**Mechanical Strength and Fatigue Performance of Laser Powder Bed Fusion Processed Hydride-dehydride Ti-6Al-4V Powders:** Mohammadreza Asherloo<sup>1</sup>; Melody Delpazir<sup>1</sup>; Ziheng Wu<sup>2</sup>; Muktesh Paliwal<sup>3</sup>; Anthony Rollett<sup>2</sup>; Amir Mostafaei<sup>1</sup>; <sup>1</sup>Illinois Institute of Technology; <sup>2</sup>Carnegie Mellon University; <sup>3</sup>Kymera International - Reading Alloys

**ENERGY**

**Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments — Fusion Materials and Metals**

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Monday AM | October 18, 2021**

**A215 | Greater Columbus Convention Center**

**Session Chairs:** Michael Short, Massachusetts Institute of Technology; Jason Trelewicz, Stony Brook University

**8:00 AM Invited**

**Real-time Thermal Oxidation Process of PFM Tungsten Under Fusion-relevant Conditions Revealed by In-situ Environmental TEM:** Maanas Togaru<sup>1</sup>; Rajat Sainju<sup>1</sup>; Lichun Zhang<sup>1</sup>; Weilin Jiang<sup>2</sup>; Yuanyuan Zhu<sup>1</sup>; <sup>1</sup>University of Connecticut; <sup>2</sup>Pacific Northwest National Laboratory

**8:20 AM Invited**

**Uncovering the Effect of Grain Boundary Dopants on Irradiation Induced Grain Growth Through In Situ Microscopy:** Jason Trelewicz<sup>1</sup>; William Cunningham<sup>1</sup>; Danny Edwards<sup>2</sup>; Yuanyuan Zhu<sup>3</sup>; <sup>1</sup>Stony Brook University; <sup>2</sup>Pacific Northwest National Laboratory; <sup>3</sup>University of Connecticut

**8:40 AM**

**Femtosecond Laser Induced Surface Damages in Tungsten and Tungsten Carbide in High Heat Flux Conditions:** Minsuk Seo<sup>1</sup>; Shukai Yu<sup>1</sup>; Venkatraman Gopalan<sup>1</sup>; Leigh Winfrey<sup>1</sup>; <sup>1</sup>The Pennsylvania State University

**9:00 AM Invited**

**Characterization of Materials Exposed to Coupled Nuclear Environments Using Positron Annihilation Spectroscopy and Electrical Impedance Spectroscopy:** Peter Hosemann<sup>1</sup>; Rasheed Auguste<sup>1</sup>; Farida Selim<sup>2</sup>; Oskar Linke<sup>3</sup>; Maik Butterling<sup>3</sup>; Hong Chan<sup>4</sup>; Junsoo Han<sup>4</sup>; Jie Qiu<sup>1</sup>; John Scully<sup>4</sup>; Ryan Schoell<sup>5</sup>; Djamel Kaoumi<sup>5</sup>; <sup>1</sup>University of California, Berkeley; <sup>2</sup>Bowling Green University; <sup>3</sup>Helmholtz Zentrum Dresden Rossendorf; <sup>4</sup>University of Virginia; <sup>5</sup>North Carolina State University

**9:20 AM**

**Richtmyer-Meshkov Instability Testing and Accompanying Analysis: A Surface Sensitive Approach to High Strain Rate Testing of Irradiated Material without Bulk Volumes:** Calvin Lear<sup>1</sup>; David Jones<sup>1</sup>; Daniel Martinez<sup>1</sup>; Jeremy Payton<sup>1</sup>; Michael Prime<sup>1</sup>; Saryu Fensin<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

**MATERIALS-ENVIRONMENT INTERACTIONS**

**Advanced Coatings for Wear and Corrosion Protection — Session I**

**Program Organizers:** Evelina Vogli, Lm Group Holdings Inc.; Virendra Singh, Schlumberger

**Monday AM | October 18, 2021**

**A220 | Greater Columbus Convention Center**

**Session Chairs:** Evelina Vogli, LM Group Holdings; Virendra Singh, Schlumberger

**8:00 AM**

**New Multidisciplinary Approach for Investigating Hot Corrosion Behavior in Thermal Barrier Coatings:** Guanlin Lyu<sup>1</sup>; JunSeong Kim<sup>1</sup>; SeungCheol Yang<sup>1</sup>; Yeon-Gil Jung<sup>1</sup>; <sup>1</sup>Changwon National University

**8:20 AM**

**Aerosol Cold Spray Technology for Ceramic and Metal Coating Deposition:** Volf Leshchynsky<sup>1</sup>; Gregorz Kubicki<sup>2</sup>; Joanna Chojnacka<sup>2</sup>; Ahmed Elseddawy<sup>1</sup>; Roman Maev<sup>1</sup>; <sup>1</sup>IDIR; <sup>2</sup>Lukasiewicz- INOP

**8:40 AM**

**Combinatorial PVD Coatings on SiC-SiC for Boiling Water Reactor Conditions:** Ryan Schoell<sup>1</sup>; Joey Kabel<sup>2</sup>; Sebastian Lam<sup>3</sup>; Amit Sharma<sup>4</sup>; Petho Laszlo<sup>4</sup>; Peter Hosemann<sup>3</sup>; Djamel Kaoumi<sup>1</sup>; <sup>1</sup>North Carolina State University; <sup>2</sup>University of California Berkeley; <sup>3</sup>University of California Berkeley; <sup>4</sup>Empa



# Technical Program

9:00 AM

**Amorphous Based PTA Weldings for Icy Surfaces:** *Evelina Vogl<sup>1</sup>*; Liang Hong<sup>2</sup>; Yan Chen<sup>2</sup>; John Kang<sup>1</sup>; Rick Salas<sup>1</sup>; <sup>1</sup>LM Group Holdings Inc.; <sup>2</sup>Texas A&M University

9:20 AM

**The Environmental Performance of Nitrided Corrosion Resistance Alloys in a Water – Glycol Hydraulic Fluid:** *Virendra Singh<sup>1</sup>*; Manuel Marya<sup>1</sup>; <sup>1</sup>Schlumberger

9:40 AM

**Properties of Ni-P-ZrC Nanocomposite Coatings for Corrosion Protection in the Oil and Gas Industry:** *Abdul Shakoor<sup>1</sup>*; Osama Fayyaz<sup>1</sup>; Ahmed Radwan<sup>1</sup>; Anwarul Hasan<sup>1</sup>; Mostafa Sleim<sup>1</sup>; Aboubakr Abdullah<sup>1</sup>; <sup>1</sup>Qatar University

10:00 AM Break

10:20 AM

**Effects of Laser Remediation Treatments on Environmentally-assisted Cracking of 5xxx Aluminum Alloys and Ship Plates:** *Yang Liu<sup>1</sup>*; Benjamin Palmer<sup>1</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University

10:40 AM

**Investigations on the Effect of Open Atmosphere Laser-nitriding on Surface Mechanical and Elevated Temperature Fretting Wear Properties of A356-Alloy:** *Achyuth Kulkarni<sup>1</sup>*; Palani I.A.<sup>1</sup>; Jayaprakash Murugesan<sup>1</sup>; <sup>1</sup>IIT Indore

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## IRON AND STEEL (FERROUS ALLOYS)

### Advancements in Steel Structural Refinement – Advancements in Steel Structural Refinement

**Sponsored by:** AIST: Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Charles Enloe, CBMM North America; Emmanuel De Moor, Colorado School of Mines; Jianfeng Wang, General Motors Global Research and Development; Jose Rodriguez-Ibabe, CEIT and TECNUN; Steven Jansto, Research and Development Resources

Monday AM | October 18, 2021

A211 | Greater Columbus Convention Center

**Session Chair:** To Be Announced

10:00 AM

**Maximizing Strengthening Mechanisms in Continuously-annealed HSLA Steel:** *Charles Enloe<sup>1</sup>*; Fabio D'Aiuto<sup>2</sup>; Hardy Mohrbacher<sup>3</sup>; <sup>1</sup>CBMM North America; <sup>2</sup>CBMM Europe; <sup>3</sup>NiobelCon bvba

10:30 AM

**Microalloyed Steel Precipitate Characterization by Automated TEM Image and EDS Analysis:** *Roger Maddalena<sup>1</sup>*; <sup>1</sup>Thermo Fisher Scientific

11:00 AM

**The Capability of Severe Plastic Deformation to Achieve High Strength and Toughness in Two High Strength Steel Alloys, Austenitic FeMnAl and Martensitic AF9628:** *Matthew Vaughan<sup>1</sup>*; Sezer Picak<sup>1</sup>; Cafer Acemi<sup>1</sup>; Richard Harris<sup>2</sup>; Peyman Samimi<sup>1</sup>; Sean Gibbons<sup>2</sup>; Rachel Abrahams<sup>2</sup>; Robert Barber<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Air Force Research Laboratory

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## ELECTRONIC AND MAGNETIC MATERIALS

### Advances in Dielectric Materials and Electronic Devices – Processing/Analysis of Dielectrics & Piezoelectrics

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Uvic, Boise State University; Matjaž Spreitzer, Jožef Stefan Institute

Monday AM | October 18, 2021

B235 | Greater Columbus Convention Center

**Session Chair:** Amar Bhalla, University of Texas at San Antonio

8:00 AM

**Unique IGa, Ta<sub>2</sub>BaTiO<sub>3</sub> Relaxor Based On Nanoscale Dipole Engineering:** *Kaijie Ning<sup>1</sup>*; Holly Shulman<sup>1</sup>; Walter Schulze<sup>1</sup>; Steven Tidrow<sup>1</sup>; <sup>1</sup>Alfred University

8:20 AM

**Zinc Oxide (ZnO): Inkjet Printing and Post-Processing Evaluation for Piezoelectric Applications:** *Sean Garnsey<sup>1</sup>*; Paul Flynn<sup>1</sup>; Bryan Gamboa<sup>1</sup>; Amar Bhalla<sup>1</sup>; Ruyan Guo<sup>1</sup>; <sup>1</sup>ECE/ COE, University of Texas at San Antonio

8:40 AM

**Electroceramics with Ferroelectric Grain Boundaries via Cold Sintering:** *Javier Mena Garcia<sup>1</sup>*; Sinan Dursun<sup>1</sup>; Kosuke Tsuji<sup>1</sup>; Sun Hwi Bang<sup>1</sup>; Zhongming Fan<sup>1</sup>; Arnaud Ndayishimiye<sup>1</sup>; Clive Randall<sup>1</sup>; <sup>1</sup>Penn State University

9:00 AM

**Production of High Temperature 3D Printed Ceramics for Sensing Applications:** *Eleanore Rogenski<sup>1</sup>*; Victoria Adams<sup>1</sup>; Eric MacDonald<sup>2</sup>; Matthew Mullin<sup>3</sup>; Ian Small<sup>3</sup>; Pedro Cortes<sup>1</sup>; <sup>1</sup>Youngstown State University; <sup>2</sup>The University of Texas at El Paso; <sup>3</sup>NASA

9:20 AM

**Effect of Deposition Humidity on the Properties of Solution-processed Indium Tin Oxide Films:** *Sivaramakrishnan Sethuraman<sup>1</sup>*; Rosario Gerhardt<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Ferrous Metallurgy — Advances in Ironmaking, Steelmaking, and Casting

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Emmanuel De Moor, Colorado School of Mines; Kishlay Mishra, Nucor Castrip Arkansas LLC; Lijia Zhao, ArcelorMittal Global R&D

**Monday AM | October 18, 2021**  
**A210 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

**8:00 AM**

**Cost Modeling and Life Cycle Analysis of Low-Emissions Iron Production:** *Muntasir Shahabuddin*<sup>1</sup>; Adam Powell<sup>1</sup>; Yan Wang<sup>1</sup>; Nikolaos Kazantzis<sup>1</sup>; Brajendra Mishra<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**8:20 AM**

**Thermodynamics and Kinetics of Coke Breeze Combustion Under Different Oxygen Content in Sintering Process:** *Dongqing Wang*<sup>1</sup>; <sup>1</sup>Shougang Group

**8:40 AM**

**The Study and Optimization of Calcium Flux for Self-fluxed Pellets:** *Xiangjuan Dong*<sup>1</sup>; Wei Wu<sup>1</sup>; Yu Cao<sup>2</sup>; Kai Wang<sup>2</sup>; Gele Qing<sup>3</sup>; Ming Li<sup>2</sup>; Wenwang Liu<sup>2</sup>; <sup>1</sup>Central Iron and Steel Research Institute; <sup>2</sup>Shougang Jingtang United Iron & Steel Co, Ltd; <sup>3</sup>Shougang Research Institute of Technology of Shougang Group Co., Ltd.

**9:00 AM**

**Structure Optimizations of Submerged Entry Nozzle in a Steel Slab Continuous Casting Mold:** *Yushi Tian*<sup>1</sup>; Lijun Xu<sup>2</sup>; Shengtao Qiu<sup>2</sup>; Rong Zhu<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Central Iron & Steel Research Institute

**9:20 AM**

**Impact of Alloy Composition on the Hot Ductility of Steel during Continuous Casting:** *Alyssa Stubbers*<sup>1</sup>; Thomas Balk<sup>1</sup>; <sup>1</sup>University of Kentucky

## ARTIFICIAL INTELLIGENCE

### AI for Big Data Problems in Advanced Imaging, Materials Modeling and Automated Synthesis — Accelerating Discovery of Materials

**Sponsored by:** TMS: Computational Materials Science and Engineering Committee

**Program Organizers:** Mathew Cherukara, Argonne National Lab; Badri Narayanan, University of Louisville; Subramanian Sankaranarayanan, University of Illinois (Chicago)

**Monday AM | October 18, 2021**  
**A124 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

**8:00 AM Invited**

**De Novo Inverse Design of Nanoporous Materials by Machine Learning:** *Mathieu Bauchy*<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

**8:30 AM Invited**

**Tuning Optoelectronic Properties of Semiconductors with First Principles Modeling and Machine Learning:** *Arun Kumar Mannodi Kanakkithodi*<sup>1</sup>; Maria Chan<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Argonne National Laboratory

**9:00 AM**

**Machine Learning Polymer Property Prediction Models with Polymers Represented as Natural Language:** *Christopher Kuenneth*<sup>1</sup>; Rampi Ramprasad<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

**9:20 AM Invited**

**Aluminum Alloy Design Using Physics Informed Machine Learning:** *Fatih Sen*<sup>1</sup>; Marat Latypov<sup>1</sup>; Heath Murphy<sup>1</sup>; Kyle Haines<sup>1</sup>; Shruthi Raj<sup>1</sup>; Aurele Mariaux<sup>2</sup>; Sazol Das<sup>1</sup>; David Anderson<sup>1</sup>; Debdutta Roy<sup>1</sup>; Yudie Yuan<sup>1</sup>; Vishwanath Hegadekatte<sup>1</sup>; <sup>1</sup>Novelis R&D Center, Kennesaw GA; <sup>2</sup>Novelis R&D Center, Sierre, Switzerland

**9:50 AM**

**Refinements to the Production of Machine Learning Interatomic Potentials:** *Jared Stimac*<sup>1</sup>; Jeremy Mason<sup>1</sup>; <sup>1</sup>University of California, Davis

**10:10 AM Break**

**10:30 AM Invited**

**Discovery of Novel Crystal Structures via Generative Adversarial Networks:** *Taylor Sparks*<sup>1</sup>; Michael Alverson<sup>1</sup>; <sup>1</sup>University of Utah

# Technical Program

## CERAMIC AND GLASS MATERIALS

### Ceramic Matrix Composites — Session I

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Narottam Bansal, NASA Glenn Research Center; Jacques Lamon, CNRS; Sung Choi, Naval Air Systems Command

**Monday AM | October 18, 2021**

**B232 | Greater Columbus Convention Center**

**Session Chair:** Marina Ruggles-Wrenn, Air Force Institute of Technology

**8:00 AM**

**Synchrotron Tomography of SiC/SiC Minicomposites to Observe and Quantify Damage Evolution:** *Ashley Hilmas<sup>1</sup>; Andrew Sharits<sup>2</sup>; Craig Przybyla<sup>1</sup>; Robert Goldberg<sup>3</sup>; Amjad Almansour<sup>3</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>UES Inc; <sup>3</sup>NASA Glenn Research Center*

**8:20 AM**

**Interfacial Fracture Toughness on SiC/SiC CMCs:** *Oriol Gavalda-Diaz<sup>1</sup>; Luc Vandeperre<sup>1</sup>; Eduardo Saiz<sup>1</sup>; Finn Giuliani<sup>1</sup>; <sup>1</sup>Imperial College London*

**8:40 AM**

**Developments in Laser-CVD to Produce SiC and Si<sub>3</sub>N<sub>4</sub> Fibers for CMC Reinforcement:** *Ram Kiran Goduguchinta<sup>1</sup>; Joseph Pegna<sup>1</sup>; Mark Schaefer<sup>1</sup>; Jeff Vervlied<sup>1</sup>; <sup>1</sup>Free Form Fibers*

**9:00 AM**

**Effectiveness of Mechanical Reinforcement of Carbon Nanotubes on Boron Carbide Through In-situ High Loading Indentation:** *Tyler Dolmetsch<sup>1</sup>; Benjamin Boesl<sup>1</sup>; Arvind Agarwal<sup>1</sup>; Cheng Zhang<sup>1</sup>; <sup>1</sup>Florida International University*

## MATERIALS-ENVIRONMENT INTERACTIONS

### Coatings to Protect Materials from Extreme Environments — Environmental and Thermal Barrier Coatings

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Kang Lee, NASA Glenn Research Center; Yutaka Kagawa, The University of Tokyo; Daniel Mumm, University of California, Irvine; Rodney Trice, Purdue University; Emmanuel Boakye, UES Inc.; Valerie Wiesner, NASA Langley Research Center; Edward Gorzkowski, Naval Research Laboratory; Scooter Johnson, Naval Research Laboratory

**Monday AM | October 18, 2021**

**A222 | Greater Columbus Convention Center**

**Session Chairs:** Rodney Trice, Purdue University; Kang Lee, NASA Glenn Research Center

**8:00 AM**

**Break-away Oxidation in Ytterbium Silicate Environmental Barrier Coatings:** *Kenneth Kane<sup>1</sup>; Eugenio Garcia<sup>2</sup>; Michael Lance<sup>1</sup>; Cory Parker<sup>1</sup>; Sanjay Sampath<sup>2</sup>; Bruce Pint<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Stony Brook University*

**8:20 AM**

**Effects of Topcoat Modifications on Bond Coat Oxidation, Internal Stresses, and Interface Toughness in Multilayer Si/Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> Environmental Barrier Coatings:** *Benjamin Herren<sup>1</sup>; Chihpin Chuang<sup>2</sup>; Jonathan Almer<sup>2</sup>; Kang Lee<sup>3</sup>; Katherine Faber<sup>1</sup>; <sup>1</sup>California Institute of Technology; <sup>2</sup>Argonne National Laboratory, Advanced Photon Source; <sup>3</sup>NASA Glenn Research Center*

**8:40 AM**

**Polymorph Stability and Thermal Expansion Tensors of Mixed and High Entropy Rare Earth Disilicates:** *Alejandro Salanova<sup>1</sup>; Rachel Guarriello<sup>1</sup>; Mackenzie Ridley<sup>1</sup>; Cormac Toher<sup>2</sup>; Stefano Curtarolo<sup>2</sup>; Elizabeth Opila<sup>1</sup>; Jon Ihlefeld<sup>1</sup>; <sup>1</sup>University of Virginia; <sup>2</sup>Duke University*

**9:00 AM**

**Evaluation of YbPO<sub>4</sub> as an Environmental Barrier Coating Candidate:** *Mackenzie Ridley<sup>1</sup>; Bohuslava McFarland<sup>2</sup>; Cameron Miller<sup>1</sup>; Elizabeth Opila<sup>1</sup>; <sup>1</sup>University of Virginia; <sup>2</sup>Pratt & Whitney*

**9:20 AM**

**Protocol for Selecting Exemplary Silicate Deposit Compositions for Evaluation of Thermal and Environmental Barrier Coatings:** *Andrew Ericks<sup>1</sup>; Frank Zok<sup>1</sup>; David Poerschke<sup>2</sup>; Carlos Levi<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>University of Minnesota*

**9:40 AM**

**High Temperature Stability and Decomposition of Mixed Oxide and Sulfate CMFAS-type Deposits and Implications for Coating Degradation:** *Eeshani Paresch Godbole<sup>1</sup>; Atharva Chikhalikar<sup>1</sup>; David Poerschke<sup>1</sup>; <sup>1</sup>University of Minnesota*

**10:00 AM Break**

**10:20 AM**

**Na<sub>2</sub>SO<sub>4</sub> Interactions with Rare Earth Silicate Environmental Barrier Coatings:** *Kristyn Ardrey<sup>1</sup>; Elizabeth Opila<sup>1</sup>; <sup>1</sup>University of Virginia*

**10:40 AM**

**Protection of Yttria Stabilized Zirconia (YSZ) Surface from CMAS Attack by Sacrificial Layer of Si<sub>3</sub>N<sub>4</sub>:** *Said Bakkar<sup>1</sup>; Elora Zucchi<sup>1</sup>; Tim Hossain<sup>2</sup>; Jacob Moldenhauer<sup>1</sup>; Ellen Steinmiller<sup>1</sup>; Will Flanagan<sup>1</sup>; <sup>1</sup>University of Dallas; <sup>2</sup>Ceriumlabs*

**11:00 AM**

**Understanding Modes of Mixed Deposit-Induced Degradation on Advanced Alloys and Bond Coat Systems:** *Atharva Chikhalikar<sup>1</sup>; Eeshani Godbole<sup>1</sup>; David Poerschke<sup>1</sup>; <sup>1</sup>University of Minnesota, Twin Cities*

## SPECIAL TOPICS

### Curricular Innovations and Continuous Improvement of Academic Programs (and Satisfying ABET along the Way): The Elizabeth Judson Memorial Symposium — Curricular Innovations and Accreditation

**Sponsored by:** TMS: Accreditation Committee, TMS: Education Committee

**Program Organizers:** Alison Polasik, Campbell University; Susan Gentry, University of California, Davis; Jeffrey Fergus, Auburn University; Assel Aitkaliyeva, University of Florida; Kester Clarke, Colorado School of Mines; Subhadra Gupta, University of Alabama; Gregg Janowski, University of Alabama at Birmingham; M. Norton, Washington State University

**Monday AM | October 18, 2021**  
**B144/145 | Greater Columbus Convention Center**

**Session Chair:** Kester Clarke, Colorado School of Mines

#### 8:00 AM Introductory Comments

#### 8:05 AM

**Changes in ABET Engineering General Criteria:** *Jeffrey Fergus*<sup>1</sup>;  
<sup>1</sup>Auburn University

#### 8:25 AM

**Preparing for an ABET Evaluation – Common Issues:** *Jeffrey Fergus*<sup>1</sup>;  
<sup>1</sup>Auburn University

#### 8:45 AM

**Universities, DOD Manufacturing Institutes and US Manufacturing-The MEEP Program:** *Cindy Waters*<sup>1</sup>; *Jeremy Chang*<sup>1</sup>; <sup>1</sup>Carderock Division Naval Surface Warfare Center

#### 9:05 AM

**A Survey of the Changes Made for Online Teaching in Materials Science and Engineering Program:** *Alison Polasik*<sup>1</sup>; *Kester Clarke*<sup>2</sup>;  
<sup>1</sup>Campbell University; <sup>2</sup>Colorado School of Mines

#### 9:25 AM Break

**9:40 AM Panel Discussion:** Assessment and Accreditation Q&A

## PROCESSING AND MANUFACTURING

### Development of Light Weight Alloys and Composites — Microstructure and Properties: Composites I

**Program Organizers:** Ramasis Goswami, Naval Research Laboratory; Nikhil Gupta, New York University; Tanjore Jayaraman, University of Michigan-Dearborn; Aashish Rohatgi, Pacific Northwest National Laboratory

**Monday AM | October 18, 2021**  
**A214 | Greater Columbus Convention Center**

**Session Chairs:** Aashish Rohatgi, PNNL; Ramasis Goswami, NRL

#### 8:00 AM Invited

**Development of a High-temperature High Strength Aluminum Alloys by Microstructure Tuning:** *Kamario Chattopadhyay*<sup>1</sup>; *Ujjval Bansal*<sup>1</sup>; *Mahender Singh*<sup>1</sup>; *Shyam Sinha*<sup>1</sup>; *Sukla Mondol*<sup>2</sup>; *Surendra Makineni*<sup>1</sup>;  
<sup>1</sup>Indian Institute of Science; <sup>2</sup>NIT Warangal

#### 8:40 AM Invited

**A Data-driven Analysis for Selection of Ti-based Alloys for Aircraft Landing Gear Beams and Future Directions:** *Tanjore Jayaraman*<sup>1</sup>; *Canumalla Ramachandra*<sup>2</sup>; <sup>1</sup>University of Michigan-Dearborn; <sup>2</sup>Weldaloy Specialty Forgings

#### 9:20 AM

**Existing and Emerging Applications of Machine Learning in Design, Synthesis, and Characterization of Metal Matrix Composites:** *Amir Kordijazi*<sup>1</sup>; *Pradeep Rohatgi*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Milwaukee

#### 9:40 AM

**Energy Efficient Solid-state Alloying and Composite Manufacturing:** *Kumar Kandasamy*; <sup>1</sup>Enabled Engineering

#### 10:00 AM Break

#### 10:20 AM Invited

**Non-Rule-of-Mixtures Thermal Diffusivity in Core-Shell-based Nanocrystalline Composite Ceramics:** *James Wollmershauser*<sup>1</sup>; *Kevin Anderson*<sup>2</sup>; *Benjamin Greenberg*<sup>2</sup>; *Heonjune Ryou*<sup>1</sup>; *Edward Gorzkowski*<sup>1</sup>; *Boris Feigelson*<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory; <sup>2</sup>National Research Council Postdoctoral Research Fellow sited at U.S. Naval Research Laboratory



# Technical Program

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## ENERGY

### Energy Materials for Sustainable Development — Energy Harvesting

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

**Monday AM | October 18, 2021**  
**A216 | Greater Columbus Convention Center**

**Session Chairs:** Kyle Brinkmann, Clemson University; Krista Carlson, University of Nevada, Reno

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**8:00 AM** Introductory Comments

**8:20 AM** Invited  
**Multi-modal Energy Harvesting-magnetic Field, Vibrations, Heat and Light:** *Shashank Priya*<sup>1</sup>; <sup>1</sup>Penn State

**8:50 AM** Invited  
**Interfacial Properties in Composite Nano-systems for Energy Harvesting:** *Alberto Vomiero*<sup>1</sup>; <sup>1</sup>Lulea University of Technology

**9:20 AM**  
**Energy Harvesting Floor from Commercial Cellulosic Materials for Self-powered Wireless Transmission Sensor System:** *Long Gu*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**9:40 AM**  
**Implanted Battery-free Direct-current Micro-power Supply from In Vivo Breath Energy Harvesting:** *Jun Li*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**10:00 AM** Break

**10:20 AM**  
**Cost-effective, Penetration/Corrosion-resistant Materials for the Containment of Earth-abundant Molten Chlorides for High-temperature Thermal Energy Storage for Concentrated Solar Power:** *Liangjuan Gao*<sup>1</sup>; *Elizabeth Laskowski*<sup>1</sup>; *Saeed Bagherzadeh*<sup>1</sup>; *Mario Caccia*<sup>1</sup>; *Michael Bichnevicius*<sup>2</sup>; *Qingzi Zhu*<sup>2</sup>; *Mehdi Pishahang*<sup>2</sup>; *Robert Cullen*<sup>3</sup>; *Kenneth McGowan*<sup>3</sup>; *Asegun Henry*<sup>3</sup>; *Kenneth Sandhage*<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Massachusetts Institute of Technology; <sup>3</sup>Westmoreland Advanced Materials, Inc.

**10:40 AM**  
**Measurement of Density for Molten Fluoride Salt:** *Jaewoo Park*<sup>1</sup>; *Jinsuo Zhang*<sup>1</sup>; <sup>1</sup>Virginia Tech

**11:00 AM**  
**Evaluation Recyclable Materials to Manufacture Wind Turbines Blades H-Darrieus:** *Andres Olivera C.*<sup>1</sup>; *Edwin Chica*<sup>1</sup>; *Henry Colorado*<sup>1</sup>; <sup>1</sup>Universidad de Antioquia

**11:20 AM**  
**Microstructure Prediction of the Laser Additive Manufacturing of Silicon-iron Soft Magnet:** *Fukang Li*<sup>1</sup>; *Kan Sun*<sup>1</sup>; *Lei Zuo*<sup>1</sup>; <sup>1</sup>Virginia Tech

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## CERAMIC AND GLASS MATERIALS

### Glasses and Optical Materials: Current Issues and Functional Applications — Dissolution and Mechanical Properties of Amorphous Solids

**Sponsored by:** ACerS Basic Science Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Delia Brauer, Otto Schott Institute of Materials Research

**Monday AM | October 18, 2021**  
**B231 | Greater Columbus Convention Center**

**Session Chair:** Douglas Meier, McCrone Associates, Inc.

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**10:00 AM**  
**X-ray Photoelectron Spectroscopy (XPS) for Improved Characterization of Glass Delamination Lamellae:** *Douglas Meier*<sup>1</sup>; <sup>1</sup>McCrone Associates, Inc.

**10:20 AM**  
**Interactive Corrosion between International Simple Glass (ISG) and Stainless Steel:** *Chandi Mohanty*<sup>1</sup>; *Xiaolei Guo*<sup>1</sup>; *Huseyin Kaya*<sup>2</sup>; *Stephane Gin*<sup>3</sup>; *Joseph Ryan*<sup>4</sup>; *John Vienna*<sup>4</sup>; *Seong Kim*<sup>5</sup>; *Jianwei Wang*<sup>6</sup>; *Jie Lian*<sup>7</sup>; *Gerald Frankel*<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>The Pennsylvania State University; <sup>3</sup>CEA; <sup>4</sup>Pacific Northwest National Laboratory; <sup>5</sup>The Pennsylvania State University; <sup>6</sup>Louisiana State University; <sup>7</sup>Rensselaer Polytechnic Institute

**10:40 AM**  
**Revisiting the Atomic Structure of Glassy Silica by Force-enhanced Atomic Refinement:** *Mathieu Bauchy*<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

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## FUNDAMENTALS AND CHARACTERIZATION

### Grain Boundaries, Interfaces, and Surfaces in Ceramics: Fundamental Structure—Property—Performance Relationships — Atomistic Approaches

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Rheinheimer Wolfgang, Forschungszentrum Jülich; Catherine Bishop, University of Canterbury; Shen Dillon, University of California, Irvine; Ming Tang, Rice University; John Blendell, Purdue University; Wayne Kaplan, Technion - Israel Institute of Technology; Melissa Santala, Oregon State University

**Monday AM | October 18, 2021**  
**B244/245 | Greater Columbus Convention Center**

**Session Chairs:** Amanda Krause, University of Florida; Wayne Kaplan, TECHNION

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**10:00 AM** Invited  
**Hetero-epitaxial Relationships and Atomic Structure at Ag/Ni Interfaces:** *Dominique Chatain*<sup>1</sup>; *Paul Wynblatt*<sup>2</sup>; *Velimir Radmilovic*<sup>3</sup>; *Ulrich Dahmen*<sup>4</sup>; <sup>1</sup>CNRS; <sup>2</sup>Carnegie Mellon University; <sup>3</sup>University of Belgrade; <sup>4</sup>Lawrence Berkeley National Laboratory

10:40 AM

**Size-dependent Lattice Contraction in Nano-MnO:** *Michael Ramsdell<sup>1</sup>; Jenna Pike<sup>2</sup>; Syed Khalid<sup>3</sup>; Siu-Wai Chan<sup>1</sup>; <sup>1</sup>Columbia University; <sup>2</sup>OxEon Energy, LLC; <sup>3</sup>Brookhaven National Laboratory*

## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Materials Discovery and Design I

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Monday AM | October 18, 2021**  
**B131 | Greater Columbus Convention Center**

**Session Chairs:** Katharine Flores, Washington University in St. Louis; Daniel Miracle, Air Force Research Laboratory

8:00 AM Invited

**Structure Design and Properties of Multiple-basis-element (MBE) Alloy Flexible Films:** Hao Huang<sup>1</sup>; Peter Liaw<sup>2</sup>; Yong Zhang<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>The University of Tennessee

8:20 AM Keynote

**High-entropy and Multi-principle Element Materials: Distinguishing Features and Emerging Opportunities:** *Daniel Miracle<sup>1</sup>; Stéphane Gorsse<sup>2</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>CNRS, University of Bordeaux*

9:00 AM Invited

**A High-throughput Strategy to Study Phase Stability and Mechanical Properties in Complex Concentrated Alloys:** Mu Li<sup>1</sup>; Zhaohan Zhang<sup>1</sup>; Arashdeep Thind<sup>1</sup>; Guodong Ren<sup>1</sup>; Rohan Mishra<sup>1</sup>; *Katharine Flores<sup>1</sup>; <sup>1</sup>Washington University in St. Louis*

9:20 AM Invited

**Computationally Guided High Entropy Alloy Discovery:** *Kenneth Smith<sup>1</sup>; John Sharon<sup>1</sup>; Ryan Deacon<sup>1</sup>; Soumalya Sarkar<sup>1</sup>; <sup>1</sup>Raytheon Technologies Research Center*

9:40 AM Invited

**Enabling High-strength and Oxidation-resistant Refractory Complex, Concentrated Alloys via Multi-fidelity Experiments and Simulations:** *Michael Titus<sup>1</sup>; <sup>1</sup>Purdue University*

## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III — Session I

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**Monday AM | October 18, 2021**  
**B246 | Greater Columbus Convention Center**

**Session Chairs:** M Arul Kumar, Los Alamos National Laboratory; Nathan Mara, University of Minnesota

8:00 AM Invited

**An Integrated Modeling-experiment Approach to Investigating Metallic Interfaces Containing 3D Character:** *Nathan Mara<sup>1</sup>; Justin Cheng<sup>1</sup>; Zezhou Li<sup>1</sup>; Shuozhi Xu<sup>2</sup>; Youxing Chen<sup>3</sup>; Jonathan Poplawsky<sup>4</sup>; Nan Li<sup>5</sup>; Irene Beyerlein<sup>2</sup>; <sup>1</sup>University of Minnesota; <sup>2</sup>University of California, Santa Barbara; <sup>3</sup>University of North Carolina, Charlotte; <sup>4</sup>Oak Ridge National Laboratory; <sup>5</sup>Los Alamos National Laboratory*

8:40 AM

**Modeling Slip Transmission across Interface Using Dislocation Dynamics Simulations:** *Aritra Chakraborty<sup>1</sup>; Abigail Hunter<sup>1</sup>; Laurent Capolungo<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory*

9:00 AM

**Confined Layer Slip in Nanolaminates: Effect of Interface Structure and Layer Thickness:** *Wurong Jian<sup>1</sup>; Shuozhi Xu<sup>1</sup>; Yanqing Su<sup>2</sup>; Irene Beyerlein<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>Utah State University*

9:20 AM

**An Investigation of the Effect of Grain Boundary Parameters on the Slip System Level Hall-petch Coefficient for Basal and Prismatic Slip Systems in Mg-4Al:** *Mohsen Taheri Andani<sup>1</sup>; Aaditya Lakshmanan<sup>1</sup>; Veera Sundararaghavan<sup>1</sup>; John Allison<sup>1</sup>; Amit Misra<sup>1</sup>; <sup>1</sup>University of Michigan*

9:40 AM

**Investigating the Mechanical Properties of Grain Boundaries with Displacement Texture Analysis:** *Anqi Qiu<sup>1</sup>; Ian Chesser<sup>2</sup>; Elizabeth Holm<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>George Mason University*

# Technical Program

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## PROCESSING AND MANUFACTURING

### Light Metal Technology — Magnesium and Joining Technology

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Xiaoming Wang, Purdue University; Yufeng Zheng, University of Nevada-Reno

**Monday AM | October 18, 2021**  
**A213 | Greater Columbus Convention Center**

**Session Chair:** Yufeng Zheng, University of Nevada-Reno

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**10:00 AM**

**Diffusion Bonding of Aluminum by applying oscillating Pressure:** Martin Salge<sup>1</sup>; Felix Gemse<sup>1</sup>; Steffen Dahms<sup>1</sup>; <sup>1</sup>Günter-Köhler-Institute GmbH

**10:20 AM**

**ECAP Strain Path Effect on Microstructure, Texture, and Mechanical Properties Evolution in Pure Magnesium:** Prakash Gautam<sup>1</sup>; Somjeet Biswas<sup>2</sup>; <sup>1</sup>India Institute of Technology Kharagpur; <sup>2</sup>IIT Kharagpur

**10:40 AM**

**Modeling and Study of the Effect of High Cooling Rates during Crystallization on the Structure and Properties of the Mg-Zr-Nd Alloy Used for Implants:** Nikita Aikin<sup>1</sup>; Vadim Shalomeev<sup>1</sup>; <sup>1</sup>Zaporozhye National Technical University

**11:00 AM**

**Ultrasonic Effects on Plastic Deformation Behavior of AA2024:** Jiarui Kang<sup>1</sup>; Randy Cheng<sup>2</sup>; Xun Liu<sup>1</sup>; Alan Taub<sup>2</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>University of Michigan

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## CERAMIC AND GLASS MATERIALS

### Manufacturing and Processing of Advanced Ceramic Materials — New Opportunities in Ceramic Processing I

**Sponsored by:** ACerS Manufacturing Division

**Program Organizers:** Bai Cui, University of Nebraska-Lincoln; James Hemrick, Oak Ridge National Laboratory; Mike Alexander, Allied Mineral Products; Eric Faierson, Quad City Manufacturing Laboratory/Western Illinois University; Keith DeCarlo, Blasch Precision Ceramics

**Monday AM | October 18, 2021**  
**B234 | Greater Columbus Convention Center**

**Session Chairs:** William Fahrenholtz, Missouri University of Science and Technology; Waltraud Kriven, University of Illinois at Urbana-Champaign

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**8:00 AM Invited**

**Recent Progress in Fusion Welding of Structural Ceramics and Composites:** William Fahrenholtz<sup>1</sup>; Greg Hilmas<sup>1</sup>; Jeremy Watts<sup>1</sup>; Jecce Jarman<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

**8:40 AM**

**Surface Strengthening of Single-crystal Alumina by High-temperature Laser Shock Peening:** Fei Wang<sup>1</sup>; Xueliang Yan<sup>1</sup>; Lei Liu<sup>1</sup>; Michael Nastasi<sup>2</sup>; Yongfeng Lu<sup>1</sup>; Bai Cui<sup>1</sup>; <sup>1</sup>University of Nebraska Lincoln; <sup>2</sup>Texas A&M University

**9:00 AM Invited**

**Low Energy Syntheses of Ceramic Powders and Composites:** Waltraud Kriven<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

**9:40 AM**

**Textured UHTC Borides Using Extremely Low Magnetic Fields:** Juan Diego Shiraishi<sup>1</sup>; Carolina Tallon<sup>2</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University; <sup>2</sup>Department of Materials Science and Engineering, Virginia Polytechnic Institute and State University

**10:00 AM Break**

**10:20 AM Invited**

**Ultra-fast Laser Sintering of Alumina and the Microstructure Prediction Based on Machine Learning:** Xiao Geng<sup>1</sup>; Jianan Tang<sup>1</sup>; Dongsheng Li<sup>2</sup>; Yunfeng Shi<sup>3</sup>; Rajendra Bordia<sup>1</sup>; Jianhua Tong<sup>1</sup>; Hai Xiao<sup>1</sup>; Fei Peng<sup>1</sup>; <sup>1</sup>Clemson University; <sup>2</sup>Advanced Manufacturing LLC; <sup>3</sup>Rensselaer Polytechnic Institute

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## MODELING

### Multi Scale Modeling of Microstructure Deformation in Material Processing — Multi Scale Modeling of Microstructure Deformation in Material Processing

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Lukasz Madej, AGH University of Science and Technology; Jaimie Tiley, Oak Ridge National Laboratory; Muszka Krzysztof, AGH University of Science and Technology; Danuta Szeliga, AGH University of Science and Technology

**Monday AM | October 18, 2021**  
**A122 | Greater Columbus Convention Center**

**Session Chair:** Xun Liu, Ohio State University

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**10:00 AM**

**Finite Element Simulation of Grain Growth with an Arbitrary Grain Boundary Energy and Explicit Grain Boundary Representation:** Erdem Eren<sup>1</sup>; Jeremy Mason<sup>1</sup>; <sup>1</sup>University of California, Davis

**10:20 AM**

**The Formation of Irradiation Induced Defects in NiTi and their Effects on the Martensitic Transformation:** Taiwu Yu<sup>1</sup>; Alejandro Hinojos<sup>1</sup>; Daniel Hong<sup>1</sup>; Peter Anderson<sup>1</sup>; Michael Mills<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>Ohio State University

**10:40 AM**

**Microstructural Evolution from Hot Torsion Tests for Material Modeling and Parameterization:** Andrew Gilmore<sup>1</sup>; Xun Liu<sup>1</sup>; <sup>1</sup>The Ohio State University

## NANOMATERIALS

### Nanotechnology for Energy, Environment, Electronics, Healthcare and Industry — Session I

**Sponsored by:** ACerS Electronics Division, TMS: Mechanical Behavior of Materials Committee

**Program Organizers:** Gary Pickrell, Virginia Tech; Navin Manjooran, Solve Technology and Research, Inc.

**Monday AM | October 18, 2021**  
**B242/243 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

**10:00 AM**

**Fabrication and Characterization of Tungsten Nanopowder for Hard Alloy Manufacturing:** *Amir Abidov<sup>1</sup>; Ahror Fattahov<sup>1</sup>; Ulugbek Ruziev<sup>1</sup>; Ilhom Asadov<sup>1</sup>; Abdullo Khursanov<sup>1</sup>; Bum Sung Kim<sup>1</sup>; Fayzullo Norkhodjaev<sup>1</sup>; <sup>1</sup>"Almalyk MMC" JSC*

**10:20 AM**

**Viral Inactivation Using Localized UV Emission and Application in Self-cleaning PPE:** *Udit Kumar<sup>1</sup>; Craig Neal<sup>1</sup>; Candace Fox<sup>1</sup>; Elayaraja Kolanthai<sup>1</sup>; Griffith Parks<sup>1</sup>; Sudipta Seal<sup>1</sup>; <sup>1</sup>University of Central Florida*

**10:40 AM**

**First-principles Study of Substituent Effects on Squaraine Dyes:** *German Barcenás<sup>1</sup>; Austin Biaggne<sup>1</sup>; Bernard Yurke<sup>1</sup>; William Knowlton<sup>1</sup>; Lan Li<sup>1</sup>; <sup>1</sup>Boise State University*

**11:00 AM**

**Ceramic Pigments of the Garnet Type Synthesized by Utilization of Rice Husk Ash:** *Irena Markovska<sup>1</sup>; Tsvetan Dimitrov<sup>2</sup>; Fila Yovkova<sup>1</sup>; <sup>1</sup>University "Prof. Dr. Asen Zlatarov" - Burgas; <sup>2</sup>Ruse University Angel Kanchev, Razgrad Branch*

## BIOMATERIALS

### Next Generation Biomaterials — Session I

**Sponsored by:** ACerS Bioceramics Division, TMS Biomaterials Committee

**Program Organizers:** Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

**Monday AM | October 18, 2021**  
**A224 | Greater Columbus Convention Center**

**Session Chairs:** Soshu Kiriha, Osaka University; Masanori Kikuchi, National Institute for Materials Science

**8:00 AM Invited**

**Controlling the Nanoscale Architecture in Rare Earth Doped Nanoparticles for Applications in Nanomedicine:** *Fiorenzo Vetrone<sup>1</sup>; <sup>1</sup>INRS, Université du Québec*

## FUNDAMENTALS AND CHARACTERIZATION

### Nucleation of Solid-State Phase Transformations — Nucleation of Solid-State Phase Transformations

**Sponsored by:** TMS Phase Transformations Committee

**Program Organizers:** Eric Lass, University of Tennessee-Knoxville; Sophie Primig, University of New South Wales; Keith Knipping, Naval Research Laboratory

**Monday AM | October 18, 2021**  
**B132 | Greater Columbus Convention Center**

**Session Chair:** Eric Lass, University of Tennessee, Knoxville

**8:00 AM Invited**

**Critical Nuclei at Hetero-phase Interfaces:** *Rongpei Shi<sup>1</sup>; Tae Wook Heo<sup>1</sup>; Brandon Wood<sup>1</sup>; Yunzhi Wang<sup>2</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>The Ohio State University*

**8:30 AM**

**Formation of the  $\gamma'$ -Ni<sub>2</sub>(Cr, Mo, W) Phase during Two-step Heat Treatment in Haynes® 244® Alloy:** *Thomas Mann<sup>1</sup>; Michael Fahrman<sup>2</sup>; Michael Titus<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Haynes International*

**8:50 AM**

**Investigation of Nucleation Mechanisms Associated with the Formation of Coprecipitates in Ni-based Superalloys:** *Hariharan Sriram<sup>1</sup>; Semanti Mukhopadhyay<sup>1</sup>; Michael Mills<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>Ohio State University*

**9:10 AM**

**Modeling Microstructure Evolution Using the Steepest-entropy-ascent Quantum Thermodynamic Framework:** *Jared McDonald<sup>1</sup>; Michael von Spakovsky<sup>2</sup>; William Reynolds<sup>2</sup>; <sup>1</sup>Virginia Polytechnic Institute; <sup>2</sup>Virginia Polytechnic Institute and State University*

**9:30 AM**

**Observing the Solid-state Processes under Additive Manufacturing Conditions Inside the TEM:** *Sriram Vijayan<sup>1</sup>; Meiyue Shao<sup>1</sup>; Avantika Gupta<sup>1</sup>; Rohan Casukhela<sup>1</sup>; Joerg Jinschek<sup>1</sup>; <sup>1</sup>The Ohio State University*



# Technical Program

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## CERAMIC AND GLASS MATERIALS

### Phase Transformations in Ceramics: Science and Applications — Experimental Studies on Structure and Control I

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Scott McCormack, University of California, Davis; Pankaj Sarin, Oklahoma State University; Sanjay V. Khare, University of Toledo; Waltraud Kriven, University of Illinois at Urbana-Champaign

**Monday AM | October 18, 2021**

**B230 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**8:00 AM Invited**

**Electrical Activation of the Martensitic Transformation in Zirconia:** *Christopher Schuh*<sup>1</sup>; Alan Lai<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**8:30 AM Invited**

**Tailorable Porous CeO<sub>2</sub>-Doped ZrO<sub>2</sub> as a Pathway to Superelastic and Shape-memory Ceramics:** Laura Quinn<sup>1</sup>; Katherine Faber<sup>1</sup>; <sup>1</sup>California Institute of Technology

**9:00 AM**

**Useful Energy Dissipation and Fatigue Resistance in Cyclically Loaded Superelastic Ceramic Granular Packings:** *Hunter Rauch*<sup>1</sup>; Joey Griffiths<sup>1</sup>; David Garcia<sup>1</sup>; Yan Chen<sup>2</sup>; Ke An<sup>2</sup>; Hang Yu<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University; <sup>2</sup>Oak Ridge National Lab

**9:20 AM**

**In-situ TEM Observation on the Motion of Phase Boundaries during Antiferroelectric Ferroelectric Transition:** *Binzhi Liu*<sup>1</sup>; Xinchun Tian<sup>1</sup>; Lin Zhou<sup>2</sup>; Xiaoli Tan<sup>1</sup>; <sup>1</sup>Iowa State University; <sup>2</sup>U.S. Department of Energy

**9:40 AM**

**Critical Parameters Controlling the Formation of High-entropy Oxides:** Kuo-Pin Tseng<sup>1</sup>; Benjamin Hulbert<sup>1</sup>; Qun Yang<sup>1</sup>; Waltraud Kriven<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

**10:00 AM Break**

**10:20 AM**

**Thermal Expansion and Phase Transformation in the Rare Earth Di-titanate System:** *Benjamin Hulbert*<sup>1</sup>; Scott McCormack<sup>2</sup>; Kuo-Pin Tseng<sup>1</sup>; Waltraud Kriven<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign; <sup>2</sup>University of California Davis

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## PROCESSING AND MANUFACTURING

### Processing and Performance of Materials Using Microwaves, Electric and Magnetic Fields, Ultrasound, Lasers, and Mechanical Work: The Rustum Roy Symposium — Session I

**Sponsored by:** ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Morsi Mahmoud, King Fahd University of Petroleum & Minerals; Dinesh Agrawal, Pennsylvania State University; Guido Link, Karlsruhe Institute of Technology; Motoyasu Sato, Chubu University; Rishi Raj, University of Colorado; Christina Wildfire, National Energy Technology Laboratory; Zhiwei Peng, Central South University

**Monday AM | October 18, 2021**

**B233 | Greater Columbus Convention Center**

**Session Chair:** Daudi Waryoba, Pennsylvania State University

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**8:00 AM**

**Assessment of Homogeneity in Percolated Composite Samples:** Miriam Rath<sup>1</sup>; Rosario Gerhardt<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

**8:20 AM**

**Freeform Microcasting:** Luciano Borasi<sup>1</sup>; Enrico Casamenti<sup>1</sup>; Raphael Charvet<sup>1</sup>; Cyril Denereaz<sup>1</sup>; Sacha Pollonghini<sup>1</sup>; Lea Deillon<sup>1</sup>; Yves Bellouard<sup>1</sup>; Andreas Mortensen<sup>1</sup>; <sup>1</sup>EPFL

**8:40 AM**

**Electromagnetic Assisted Thermal Processing Enabling Spatially Selective Phase Transformation of Metal Amorphous Nanocomposites:** *Ahmed Talaat*<sup>1</sup>; Kevin Byerly<sup>2</sup>; David Greve<sup>2</sup>; Michael McHenry<sup>2</sup>; Paul Ohodnicki<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Carnegie Mellon University

**9:00 AM**

**Solid State Joining of Dissimilar Single Crystal Ni-based Superalloys Using Field Assisted Sintering Technology (FAST):** *Charis Lin*<sup>1</sup>; Jogender Singh<sup>1</sup>; Matthew Hogan<sup>1</sup>; Namiko Yamamoto<sup>1</sup>; <sup>1</sup>The Pennsylvania State University

**9:20 AM Invited**

**Electric Current Processing of Additively Manufactured Ti-6Al-4V Alloy:** *Daudi Waryoba*<sup>1</sup>; Zahabul Islam<sup>1</sup>; Ted Reutzel<sup>1</sup>; Aman Haque<sup>1</sup>; <sup>1</sup>Pennsylvania State University

## MATERIALS-ENVIRONMENT INTERACTIONS

### Thermodynamics of Materials in Extreme Environments — Thermodynamics of Nuclear Materials and Minerals

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division

**Program Organizers:** Xiaofeng Guo, Washington State University; Kristina Lilova, Arizona State University; Kyle Brinkman, Clemson University; Alexandra Navrotsky, Arizona State University; Jake Amoroso, Savannah River National Laboratory; Xingbo Liu, West Virginia University; Gustavo Costa, NASA Glenn Research Center

**Monday AM | October 18, 2021**  
**A221 | Greater Columbus Convention Center**

**Session Chairs:** Xiaofeng Guo, Washington State University; Kyle Brinkman, Clemson University

#### 8:00 AM Introductory Comments

#### 8:10 AM Invited

**ACerS Navrotsky Award for Experimental Thermodynamics of Solids: Advancing Solar-Driven Thermochemical Fuel Production Using Nonstoichiometric Perovskites:** *Xin Qian*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

#### 8:55 AM

**Thermodynamic Investigation of Multicomponent Chloride Molten Salts for Spent Fuel Processing:** *Liangyan Hao*<sup>1</sup>; Soumya Sridar<sup>1</sup>; Elizabeth Sooby<sup>2</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>University of Texas at San Antonio

#### 9:15 AM Invited

**Energetics of Fe<sub>3</sub>O<sub>4</sub> – FeAl<sub>2</sub>O<sub>4</sub> Spinel Solid Solution:** *Alexandra Navrotsky*<sup>1</sup>; <sup>1</sup>Arizona State University

## PROCESSING AND MANUFACTURING

### 13th Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing — Novel Approaches to Sustainable Manufacturing I

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Surojit Gupta, University of North Dakota; Rajiv Asthana, University of Wisconsin; Hisayuki Suematsu, Nagaoka University of Technology; Mritunjay Singh, Ohio Aerospace Institute; Enrico Bernardo, University of Padova; Yiquan Wu, Alfred University; Zhengyi Fu, Wuhan University of Technology; Allen Apblett, Oklahoma State University; Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology

**Monday PM | October 18, 2021**  
**A212 | Greater Columbus Convention Center**

**Session Chairs:** Huong Le, Faraday Technology; Kathy Lu, Virginia Polytechnic Institute and State University

#### 2:00 PM

**Continuous Electrochemical Destruction of Contaminants of Emerging Concern (CECs) for Wastewater Treatment:** *Huong Le*<sup>1</sup>; Rajes Radhakrishnan<sup>1</sup>; Brian Skinn<sup>1</sup>; Timothy D Hall<sup>1</sup>; Stephen Snyder<sup>1</sup>; E. Jennings Taylor<sup>1</sup>; Maria Inman<sup>1</sup>; Chris Athmer<sup>2</sup>; <sup>1</sup>Faraday Technology; <sup>2</sup>Terran Corporation

#### 2:20 PM

**Design of Novel Electrocoagulation Systems for Produced Water Treatment:** *Stephen Polkowski*<sup>1</sup>; Pankaj Sarin<sup>1</sup>; <sup>1</sup>Oklahoma State University

#### 2:40 PM

**Microstructural Evolution and Mechanical Properties of Shear Assisted Processing and Extrusion (ShAPE) Processed Aluminum Alloys:** *Rajib Kalsar*<sup>1</sup>; Xiaolong Ma<sup>1</sup>; Jens Darsell<sup>1</sup>; Miao Song<sup>1</sup>; Nicole Overman<sup>1</sup>; Keerti Kappagantula<sup>1</sup>; Vineet Joshi<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

#### 3:00 PM

**Performance Assessment of Sustainable Near-dry EDM Process during Machining of Micro-channels on Ni-Ti Based Shape Memory Alloys:** Ramver Singh<sup>1</sup>; Akshay Divvedi<sup>1</sup>; Pradeep Kumar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (IIT), Roorkee

#### 3:20 PM Break

#### 3:40 PM

**Vibration and Mechanical Analysis of FDM Manufactured Soybean Hull Fiber/Polymer Composites:** *Roshan Mishra*<sup>1</sup>; Osama Sultan Bu Aamiri<sup>1</sup>; Saleh Khanjar<sup>1</sup>; Kunal Kate<sup>1</sup>; Jagannadh Satyavolu<sup>1</sup>; <sup>1</sup>University of Louisville

#### 4:00 PM

**Design of Novel Materials from Corn-based Precursors:** *Surojit Gupta*<sup>1</sup>; <sup>1</sup>University of North Dakota

# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — AM Modeling - Mechanical Properties

**Sponsored by:** TMS Computational Materials Science and Engineering Committee

**Program Organizers:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

**Monday PM | October 18, 2021**  
**A113 | Greater Columbus Convention Center**

**Session Chairs:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, CCDC Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeon-Gil Jung, Changwon National University

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**2:00 PM**

**Grain-scale Residual Stress Modeling in Wire Arc Additive Manufacturing of Haynes 282 Super Alloy:** *Santanu Paul<sup>1</sup>; Wei Xiong<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**2:20 PM**

**Influence of Microstructure on Fatigue Crack Growth: An Combined Experiment and Model Investigation in EBM Nickel-Based Supper Alloy Haynes 282:** *Jiahao Cheng<sup>1</sup>; Patxi Fernandez-Zelaia<sup>1</sup>; Sebastien Dryepont<sup>1</sup>; Xiaohua Hu<sup>1</sup>; Michael Kirka<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

**2:40 PM**

**Part-level Fast Predictions of Residual Stresses during LPBF of Al-Mg-Zr Alloys Using Microstructure Informed Inherent Strain Method:** *Abhishek Ramakrishnan<sup>1</sup>; Daniel Satko<sup>1</sup>; Ayman Salem<sup>1</sup>; Jan Kasprzak<sup>2</sup>; Nam Phan<sup>2</sup>; <sup>1</sup>MRL Materials Resources LLC; <sup>2</sup>Naval Air Systems Command*

**3:00 PM**

**Distortion Modeling during Sintering of Binder Jet Printed Parts:** *Basil Paudel<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**3:20 PM Break**

**3:40 PM**

**Modeling and Experimental Validation of Stresses in 3D Printed, Polymeric Biliary Stents:** *Victoria Cordista<sup>1</sup>; Rebecca Lawson<sup>1</sup>; Bailey Stanley<sup>1</sup>; Sagar Patel<sup>1</sup>; Joanna Thomas<sup>1</sup>; <sup>1</sup>Mercer University*

**4:00 PM**

**Residual Stress Induced Cracking Modeling:** *Kevin Glunt<sup>1</sup>; Wen Dong<sup>1</sup>; Santanu Paul<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**4:20 PM**

**Improving the Mechanical Performance of AlSi10Mg Lattice Structures Manufactured by Laser Powder Bed Fusion (L-PBF):** *Hend Alqaydi<sup>1</sup>; Sultan Alneyadi<sup>2</sup>; Jide Oyeboji<sup>1</sup>; Dong Lee<sup>1</sup>; Nesma Aboulkhair<sup>1</sup>; <sup>1</sup>Technology Innovation Institute; <sup>2</sup>Pennsylvania state university*

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Ceramic-based Materials: Process Development, Materials, Process Optimization and Applications — Session II: Extrusion-based AM and Stereolithography

**Sponsored by:** ACerS Engineering Ceramics Division, ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Xuan Song, University of Iowa; Lei Chen, University of Michigan-Dearborn; Xiangyang Dong, Missouri University of Science and Technology; Yiquan Wu, Alfred University; Paolo Colombo, University of Padova; Rajendra Bordia, Clemson University; Long-Qing Chen, Pennsylvania State University

**Monday PM | October 18, 2021**  
**A112 | Greater Columbus Convention Center**

**Session Chairs:** Yiquan Wu, Alfred University; Xuan Song, University of Iowa

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**2:00 PM**

**Multifunctional Artificial Artery from Direct 3D Printing with Built-in Ferroelectricity and Tissue-Matching Modulus:** *Jun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison*

**2:20 PM**

**Direct-write 3D Printing of Electrodes for High Power Density Batteries:** *Amjad Almansour<sup>1</sup>; Mrityunjay Singh<sup>2</sup>; Michael Halbig<sup>1</sup>; Daniel Gorican<sup>3</sup>; <sup>1</sup>NASA Glenn Research Center; <sup>2</sup>Ohio Aerospace Institute at NASA Glenn Research Center; <sup>3</sup>HX5, LLC at NASA Glenn Research Center*

**2:40 PM Invited**

**The Influence of Processing on the Mechanical Properties of Additively Manufactured Ceramic Matrix Composites:** *Mark O'Masta<sup>1</sup>; Ekaterina Stonkevitch<sup>1</sup>; Kaleigh Porter<sup>1</sup>; Phuong Bui<sup>1</sup>; Natalie Larson<sup>2</sup>; Zak Eckel<sup>1</sup>; Tobias Schaedler<sup>1</sup>; <sup>1</sup>HRL Laboratories LLC; <sup>2</sup>Harvard University*

**3:10 PM**

**Additive Manufacturing of Yttrium-stabilized Zirconia Architectures with Stretch-dominated Mechanical Properties:** *Hunter Rauch<sup>1</sup>; Kendall Knight<sup>1</sup>; Huachen Cui<sup>2</sup>; Jake Yoder<sup>1</sup>; Xiaoyu Zheng<sup>2</sup>; Hang Yu<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University; <sup>2</sup>University of California, Los Angeles*

**3:30 PM Break**

**3:50 PM**

**Characterization of Anisotropic Structure of Additive Manufactured Ceramics:** *Rosario Gerhard<sup>1</sup>; Yifan Jin<sup>1</sup>; Zev Greenberg<sup>1</sup>; Shawn Allan<sup>2</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>Lithoz America, LLC*

**4:10 PM Invited**

**3D Printing of Nd:YAG Laser Ceramics through Lithography-based Light Projection:** *Guangran Zhang<sup>1</sup>; Yiquan Wu<sup>1</sup>; <sup>1</sup>Alfred University*

**4:40 PM**

**Enhanced Piezocomposite Transducers with 3D Printed Piezoelectric PZT:** *Shawn Allan<sup>1</sup>; Nicholas Voellm<sup>1</sup>; Justin Tufariello<sup>2</sup>; Barry Robinson<sup>3</sup>; Alex Angilella<sup>2</sup>; Leslie Riesenhuber<sup>2</sup>; Brian Pazol<sup>3</sup>; <sup>1</sup>Lithoz America LLC; <sup>2</sup>The MITRE Corporation; <sup>3</sup>MSI Transducers Corp.*

**5:00 PM**

**Stereolithography Printing of Technical Ceramics and Its Applications:**  
*Kenna Ritter<sup>1</sup>; Peter Durcan<sup>1</sup>; 13DCERAM SINTO INC*

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#### ADDITIVE MANUFACTURING

**Additive Manufacturing of High and Ultra-High Temperature Ceramics and Composites: Processing, Characterization and Testing — Binder Jet 3D Printing, Post-processing, and Testing**

*Sponsored by:* ACerS Engineering Ceramics Division

**Program Organizers:** Corson Cramer, Oak Ridge National Laboratory; Greg Hilmas, Missouri University of Science and Technology; Lisa Rueschhoff, Air Force Research Laboratory

**Monday PM | October 18, 2021**

**A111 | Greater Columbus Convention Center**

**Session Chair:** William Costakis, Air Force Research Labs

**4:00 PM Invited**

**Binder Jet Additive Manufacturing of Novel Design, High Temperature, Ceramic Heat Exchangers:** *Benjamin Groth<sup>1</sup>; Jesse Blacker<sup>1</sup>; 1ExOne*

**4:40 PM**

**Oxidation of 3D-printed SiC in Air and Steam Environments:** *Kenneth Kane<sup>1</sup>; Padraig Stack<sup>2</sup>; Danny Schappel<sup>1</sup>; Katherine Montoya<sup>3</sup>; Peter Mouche<sup>1</sup>; Elizabeth Sooby<sup>3</sup>; Kurt Terrani<sup>1</sup>; 1Oak Ridge National Laboratory; 2University of Akron; 3University of Texas*

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#### ADDITIVE MANUFACTURING

**Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Ni-based Alloys**

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

**Monday PM | October 18, 2021**

**A115 | Greater Columbus Convention Center**

**Session Chair:** Ian Nettleship, University of Pittsburgh

**2:00 PM**

**Creation of Process Representative Flaws and Their Impact on the Mechanical Properties L-PBF Inconel 718:** *Jacob Rindler<sup>1</sup>; David Schick<sup>2</sup>; Peter Daum<sup>3</sup>; Adam Sutton<sup>4</sup>; Michael Groeber<sup>1</sup>; 1Ohio State University; 2Proto Precision Additive; 3Rolls Royce; 4Lockheed Martin*

**2:20 PM**

**The Material Quality of Samples Obtained by Selective Laser Melting Method from IN718 Alloy Powder:** *Vladimir Klochikhin<sup>1</sup>; Pavel Kasay<sup>1</sup>; Konstantin Balushok<sup>1</sup>; Valeriy Shilo<sup>1</sup>; Valeriy Naumyk<sup>2</sup>; 1JSC «Motor Sich»; 2NU «Zaporizhzhya Polytechnic»*

**2:40 PM**

**Heat Treatment Design of Haynes 282 Alloy Prepared by Wire-arc Additive Manufacturing:** *Yuankang Wang<sup>1</sup>; Rafael Rodriguez De Vecchis<sup>1</sup>; Wei Xiong<sup>1</sup>; 1University of Pittsburgh*

**3:00 PM**

**Microstructure Development of Additively Manufactured Gamma Prime Strengthened Ni-based Superalloy Rene65:** *Colleen Hilla<sup>1</sup>; Andrew Wessman<sup>2</sup>; Alber Sadek<sup>3</sup>; Hyeyun Song<sup>4</sup>; Wei Zhang<sup>1</sup>; Michael Mills<sup>1</sup>; 1Ohio State University; 2University of Arizona; 3Edison Welding Institute; 4Edison Welding Institute*

**3:20 PM Break**

**3:40 PM**

**Print Defects, Microstructure Evolution and Remnant Porosity for Binder-jet Printed 625 Alloy:** *Chuyuan Zheng<sup>1</sup>; Ian Nettleship<sup>1</sup>; Markus Chmielusz<sup>1</sup>; 1University of Pittsburgh*

**4:00 PM**

**Mechanical Behavior of Ni-based Superalloy Single Crystals Produced via Electron Beam Melting AM:** *Patxi Fernandez-Zelai<sup>1</sup>; Quinn Campbell<sup>1</sup>; Chris Ledford<sup>1</sup>; Michael Kirka<sup>1</sup>; Sebastien Dreypondt<sup>1</sup>; 1Oak Ridge National Laboratory*

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#### ADDITIVE MANUFACTURING

**Additive Manufacturing of Metals: ICME Gaps: Material Property and Validation Data to Support Certification — Data Acquisition: Material Property and Validation Data to Support Certification**

*Sponsored by:* TMS: Integrated Computational Materials Engineering Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Joshua Fody, NASA Langley Research Center; Edward Glaessgen, NASA Langley Research Center; Christopher Lang, NASA Langley Research Center; Greta Lindwall, KTH Royal Institute of Technology; Michael Sansoucie, NASA Marshall Space Flight Center; Mark Stoudt, National Institute of Standards and Technology

**Monday PM | October 18, 2021**

**A114 | Greater Columbus Convention Center**

**Session Chairs:** Jonathan Raush, University of Louisiana at Lafayette; Michael Sansoucie, NASA

**2:00 PM**

**High Temperature Material Properties Measurement Capabilities of the NASA MSFC Electrostatic Levitation (ESL) Laboratory:** *Michael Sansoucie<sup>1</sup>; 1NASA Marshall Space Flight Center*

**2:20 PM Invited**

**Laser Energy Coupling during Metal Additive Manufacturing:** *Brian Simonds<sup>1</sup>; 1NIST*

**2:50 PM**

**An Analysis of the Dislocation Density of Inconel 718 Additive Manufacturing Powder:** *Colby Azersky<sup>1</sup>; Sangho Jeon<sup>2</sup>; Peggy Cebe<sup>3</sup>; 1NASA; 2Korea Research Institute of Standards and Science; 3Tufts University*

**3:10 PM Keynote**

**Providing a Rigorous Measurement Foundation for Modeling-Informed Qualification and Certification of Metal AM Components:** *Lyle Levine<sup>1</sup>; Brandon Lane<sup>1</sup>; Thien Phan<sup>1</sup>; Fan Zhang<sup>1</sup>; Mark Stoudt<sup>1</sup>; Brian Simonds<sup>1</sup>; David Deisenroth<sup>1</sup>; 1National Institute of Standards and Technology*



# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Advanced Characterization for Industrial Applications — Structures and Material Properties

**Sponsored by:** TMS Advanced Characterization, Testing, and Simulation Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Nadia Kouraytem, Utah State University; Fan Zhang, National Institute of Standards and Technology; Lianyi Chen, University of Wisconsin-Madison

**Monday PM | October 18, 2021**  
**A121 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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#### 2:00 PM Invited

**Synchrotron Characterization of Hot Cracking and Related Topics:** *Anthony Rollett*<sup>1</sup>; Guannan Tang<sup>1</sup>; Nadia Kouraytem<sup>2</sup>; Benjamin Gould<sup>3</sup>; Joseph Pauza<sup>4</sup>; Ziheng Wu<sup>1</sup>; Joseph Aroh<sup>1</sup>; Runbo Jiang<sup>1</sup>; Seunghee Oh<sup>1</sup>; Srujana Yarasi<sup>1</sup>; Ann Choi<sup>1</sup>; Amit Verma<sup>1</sup>; Rajib Halder<sup>1</sup>; Andrew Huck<sup>1</sup>; Zhening Yang<sup>1</sup>; Amaranth Karra<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Utah State University; <sup>3</sup>Argonne National Laboratory

#### 2:30 PM

**Moisture Impacts in AM Metal Powders Characterized by Karl Fischer Oven Titration and Avalanche Rheometry:** *Dave van der Wiel*<sup>1</sup>; Ethan Pawlak<sup>1</sup>; Tyler Gutzky<sup>1</sup>; <sup>1</sup>NSL Analytical

#### 2:50 PM

**Investigation of the Protective Mixture Influence on the Heat Input Meaning for the Layered Electric Arc Surfacing of Aluminum Alloys AlSi5 and AlMg5:** Mikhail Gnatenko<sup>1</sup>; *Valeriy Naumyk*<sup>2</sup>; Maria Matkovska<sup>2</sup>; Vadim Shalomoev<sup>2</sup>; <sup>1</sup>JSK Motor Sich; <sup>2</sup>NU "Zaporizhzhya Polytechnic"

#### 3:10 PM

**Gradient Alloy Heat Exchanger Manufacturing for Energy Applications:** Kevin Luo<sup>1</sup>; Bob Markley<sup>2</sup>; Nadia Kouraytem<sup>3</sup>; Hailei Wang<sup>3</sup>; *Michael Juhasz*<sup>4</sup>; <sup>1</sup>Formalloy Technologies, Inc.; <sup>2</sup>3rd Dimension Industrial 3D Printing Co; <sup>3</sup>Utah State University; <sup>4</sup>FormAlloy Technologies, Inc.

#### 3:30 PM Break

#### 3:50 PM

**Tensile Behavior of Metal AM Lattice Structures:** *Benedict DiMarco*<sup>1</sup>; Jeremy Seidt<sup>1</sup>; Ariel Gluck; Jacob Rindler<sup>1</sup>; Edward Herderick<sup>1</sup>; <sup>1</sup>The Ohio State University

#### 4:10 PM

**The Effect of the Cross-sectional Area on the Microstructure and Mechanical Properties of AlSi10Mg Parts Manufactured by Laser Powder Bed Fusion (L-PBF):** *Nujood Alshehhi*<sup>1</sup>; Lewis Kindleyside<sup>2</sup>; Nesma Aboulkhair<sup>1</sup>; <sup>1</sup>TII; <sup>2</sup>Khalifa University

#### 4:30 PM

**The Influence of the Characteristic Microstructure of Additively Manufactured AlSi10Mg on the Mechanical Behaviour at Various Strain Rates:** *Natalia Ghis*<sup>1</sup>; Henrique Ramos<sup>1</sup>; Rafael Santiago<sup>1</sup>; Lewis Kindleyside<sup>2</sup>; Wesley Cantwell<sup>2</sup>; Nesma Aboulkhair<sup>3</sup>; <sup>1</sup>TII; <sup>2</sup>Khalifa University; <sup>3</sup>University of Nottingham

#### 4:50 PM Concluding Comments

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — Session II

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**Monday PM | October 18, 2021**  
**A120 | Greater Columbus Convention Center**

**Session Chair:** Anthony Rollett, Carnegie Mellon University

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#### 4:00 PM

**An Automated Tool for Porosity Characterization and Classification in LPBF:** Evan Diewald<sup>1</sup>; *Jack Beuth*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

#### 4:20 PM

**Time-resolved Characterization of Evolving Phase and Microstructure of Ti-6Al-4V during Laser Processing with Synchrotron X-ray Diffraction:** *Seunghee Oh*<sup>1</sup>; Rachel Lim<sup>2</sup>; Joseph Aroh<sup>1</sup>; Andrew Chuang<sup>3</sup>; Benjamin Gould<sup>3</sup>; Behnam Amin-Ahmadi<sup>4</sup>; Joel Bernier<sup>5</sup>; Tao Sun<sup>6</sup>; P. Chris Pistorius<sup>1</sup>; Robert Suter<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Penn State University; <sup>3</sup>Argonne National Laboratory; <sup>4</sup>Colorado School of Mines; <sup>5</sup>Lawrence Livermore National Laboratory; <sup>6</sup>University of Virginia

#### 4:40 PM

**Modeling of True Stress-Strain in the Plastic Regime of Additively Manufactured Ti-6Al-4V:** *Andrew Temple*<sup>1</sup>; Maria Quintana<sup>1</sup>; Peter Collins<sup>1</sup>; <sup>1</sup>Iowa State University

#### 5:00 PM

**On the Use of Energy Dispersive Spectroscopy to Inform on Local Property Variations and Defect Formation across AM Processes:** *Katie O'Donnell*<sup>1</sup>; Maria Quintana<sup>1</sup>; Matthew Kenney<sup>1</sup>; Andrew Temple<sup>1</sup>; Scott Blazanin<sup>1</sup>; Shraddha Vachhani<sup>1</sup>; Peter Collins<sup>1</sup>; <sup>1</sup>Iowa State University

#### 5:20 PM

**Reactivating Transformation Induced Plasticity (TRIP) in an Additively Manufactured  $\beta$ -Ti Alloy:** *Srinivas Aditya Mantri*<sup>1</sup>; MSKKY Nartu<sup>1</sup>; Narendra Dahotre<sup>1</sup>; Rajarshi Banerjee<sup>1</sup>; <sup>1</sup>University of North Texas

## ENERGY

### Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments — Nuclear Fuels, Ceramics, and Corrosion

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Monday PM | October 18, 2021**  
**A215 | Greater Columbus Convention Center**

**Session Chairs:** Marat Khafizov, Ohio State University; Christopher Barr, US Naval Nuclear Laboratory

#### 2:00 PM Invited

**Characterization of Defects, Thermal Transport, and Elastic Properties in As-fabricated and Irradiated Single Crystal of ThO<sub>2</sub>:** *Marat Khafizov*<sup>1</sup>; *Saqeeb Adnan*<sup>1</sup>; *Joshua Ferrigno*<sup>1</sup>; *Vinay Chauhan*<sup>1</sup>; *Amey Khanolkar*<sup>2</sup>; *Cody Dennett*<sup>2</sup>; *Yuzhou Wang*; *Kaustubh Bawane*<sup>2</sup>; *Linu Malakkal*<sup>2</sup>; *Miaomiao Jin*<sup>3</sup>; *Zilong Hua*<sup>2</sup>; *Chao Jiang*<sup>2</sup>; *Lingfeng He*<sup>2</sup>; *Chris Marianetti*<sup>4</sup>; *Anter El-Azab*<sup>5</sup>; *David Hurley*<sup>2</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Idaho National Laboratory; <sup>3</sup>Pennsylvania State University; <sup>4</sup>Columbia University; <sup>5</sup>Purdue University

#### 2:20 PM Invited

**In Situ Ion Irradiation of Gadolinium Titanate: A Perspective on Microstructure and Memory:** *Jessica Krogstad*<sup>1</sup>; *Nathan Madden*<sup>1</sup>; *Matthew Janish*<sup>2</sup>; *James Valdez*<sup>2</sup>; *Blas Uberuaga*<sup>2</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign; <sup>2</sup>Los Alamos National Laboratory

#### 2:40 PM

**Insight into the Impact of Irradiation on Vibrational Properties of AlN Using Raman Spectroscopy:** *Saqeeb Adnan*<sup>1</sup>; *Yuzhou Wang*<sup>2</sup>; *Aleksandr Chernatynskiy*<sup>3</sup>; *Marat Khafizov*<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Idaho National Laboratory; <sup>3</sup>Missouri University of Science and Technology

#### 3:00 PM

**Optical Characterization of Defects in Proton Irradiated Fluorite Oxides:** *Joshua Ferrigno*<sup>1</sup>; *Vinay Chauhan*<sup>1</sup>; *Amey Khanolkar*<sup>2</sup>; *Lingfeng He*<sup>2</sup>; *David Hurley*<sup>2</sup>; *Marat Khafizov*<sup>1</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Idaho National Laboratory

#### 3:20 PM

**Microstructural Characterization of Oxidized Tristructural Isotropic Particles (TRISO) in Various Gas Atmospheres:** *Katherine Montoya*<sup>1</sup>; *Brian Brigham*<sup>1</sup>; *Tyler Gerczak*<sup>2</sup>; *Elizabeth Sooby*<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio; <sup>2</sup>Oak Ridge National Laboratory

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Coatings for Wear and Corrosion Protection — Session II

**Program Organizers:** Evelina Vogli, Lm Group Holdings Inc.; Virendra Singh, Schlumberger

**Monday PM | October 18, 2021**  
**A220 | Greater Columbus Convention Center**

**Session Chairs:** Evelina Vogli, LM Group Holdings; Virendra Singh, Schlumberger

#### 2:00 PM

**The Effects of Graphene in Composite Polymer Coatings Against Inorganic Scales:** *Manuel Marya*<sup>1</sup>; *Virendra Singh*<sup>1</sup>; *Alireza Zolfaghari*<sup>1</sup>; <sup>1</sup>Schlumberger

#### 2:20 PM

**Direct Electrodeposition of Corrosion Resistant Coatings onto Aluminum Alloys:** *Rajeswaran Radhakrishnan*<sup>1</sup>; *Timothy Hall*<sup>1</sup>; *Maria Inman*<sup>1</sup>; *Earl Jennings Taylor*<sup>1</sup>; *Stephen Snyder*<sup>1</sup>; *Cory Crowley*<sup>2</sup>; <sup>1</sup>Faraday Technology Inc; <sup>2</sup>Fermi National Accelerator Laboratory

#### 2:40 PM

**Improved Coating Performance of REACH Compliant Trivalent Chromium Plating Process for Functional Applications:** *Andrew Moran*<sup>1</sup>; *Tim Hall*<sup>1</sup>; *Rajeswaran Radhakrishnan*<sup>1</sup>; *Stephen Snyder*<sup>1</sup>; *Maria Inman*<sup>1</sup>; *EJ Taylor*<sup>1</sup>; *Kamyar Ahmadi*<sup>2</sup>; *Stanko Brankovic*<sup>2</sup>; *George Bokisa*<sup>3</sup>; *Mark Feathers*<sup>4</sup>; <sup>1</sup>Faraday Technology Inc.; <sup>2</sup>University of Houston; <sup>3</sup>Coventry International; <sup>4</sup>U.S. Army Aviation and Missile Command

#### 3:00 PM

**Galvanic Corrosion Mitigation of CFRP-AZ31B Dissimilar Joint:** *Yong Chae Lim*<sup>1</sup>; *Jiheon Jun*<sup>1</sup>; *Jong Kahk Keum*<sup>1</sup>; *Yuan Li*<sup>1</sup>; *Donovan Leonard*<sup>1</sup>; *Michael Brady*<sup>1</sup>; *Zhili Feng*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

#### 3:20 PM Break

#### 3:40 PM

**Novel Spray-on TBC Coating with Outstanding Wear and Corrosion Protection:** *Paul Curtis*<sup>1</sup>; <sup>1</sup>Applied Thin Films, Inc.

#### 4:00 PM

**Polymeric Coatings Embedded with Green Anti-corrosive Pigment for Corrosion Inhibition of Steel:** *Muddasir Nawaz*<sup>1</sup>; *Abdul Shakoor*<sup>1</sup>; *Ramazan Kahraman*<sup>1</sup>; *M. F. Montemor*<sup>2</sup>; <sup>1</sup>Qatar University; <sup>2</sup>Universidade de Lisboa

#### 4:20 PM

**Controlled Release of Corrosion Inhibitors by Microencapsulation for Protection of Steel Reinforced Concrete:** *Jacob Ressa*<sup>1</sup>; *David Bastidas*<sup>1</sup>; *Ulises Martin*<sup>1</sup>; *Juan Bosch*<sup>1</sup>; <sup>1</sup>University of Akron

#### 4:40 PM

**High-performance Chrome Coatings to Protect Against Wear and Corrosion:** *Borys Sereda*<sup>1</sup>; *Dmytro Sereda*<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

# Technical Program

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Session I

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**Monday PM | October 18, 2021**  
**A223 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

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**2:00 PM**

**Investigation of the Variables Affecting Hot Corrosion Test Results:** Preston Nguyen<sup>1</sup>; Brian Gleeson<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**2:20 PM**

**Characterization and High Temperature Electrical Properties of Brazed Joints of La<sub>0.8</sub>Sr<sub>0.2</sub>CrO<sub>3</sub> with Nickel and Nickel Alloys:** Zhengtao Yang<sup>1</sup>; Javier Mena<sup>1</sup>; Jordan Conte<sup>1</sup>; Brian Jordan<sup>1</sup>; Katarzyna Sabolsky<sup>1</sup>; Kostas Sierros<sup>1</sup>; Edward Sabolsky<sup>1</sup>; <sup>1</sup>West Virginia University

**2:40 PM**

**Determining the Effect of Aerospace Environments on the Corrosion Fatigue Performance of AA7085-T7451:** Brandon Free<sup>1</sup>; Sarah Galyon Dorman<sup>2</sup>; Jason Niebuhr<sup>2</sup>; Nathan Houser<sup>2</sup>; Jenifer Locke<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>SAFE Inc.

**3:00 PM**

**Economically Alloyed High-speed Steel for Knives of Feeder Feeders of Glass Forming Machines:** Valeriy Mishchenko<sup>1</sup>; Sergiy Sheyko<sup>1</sup>; Vldimir Tsyganov<sup>2</sup>; Olha Bolsun<sup>1</sup>; Svitlana Mudra<sup>1</sup>; <sup>1</sup>Zaporizhzhia National University; <sup>2</sup>National University "Zaporizhzhia Polytechnic"

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## ELECTRONIC AND MAGNETIC MATERIALS

### Advances in Dielectric Materials and Electronic Devices — Magnetic Materials

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Ubc, Boise State University; Matjaž Spreitzer, Jožef Stefan Institute

**Monday PM | October 18, 2021**  
**B235 | Greater Columbus Convention Center**

**Session Chair:** Amar Bhalla, University of Texas at San Antonio

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**2:00 PM**

**Magnetocaloric Composites for High Efficiency Thermal Management:** Christopher Kovacs<sup>1</sup>; Timothy Haugan<sup>2</sup>; Michael McLeod<sup>3</sup>; Devin Grant<sup>4</sup>; <sup>1</sup>Scintillating Solutions LLC; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>University of Dayton Research Institute; <sup>4</sup>Central State University

**2:20 PM**

**Improvement of the Magnetic Characteristics of Materials Due to the Formation of Unidirectional Boundaries of Ferrite during Processing in SHS Conditions:** Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Vitalyy Volokh<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

**2:40 PM**

**The influence of the Microstructure Obtained After Processing in SHS Conditions on the Magnetic Characteristics of Steels:** Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Vitalyy Volokh<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

**3:00 PM**

**The Effect of Deformation of Low Alloy Steels Used in Metallurgy on Their Magnetic Characteristics:** Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Vitalyy Volokh<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

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## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Ferrous Metallurgy — Advances in Steel Products

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Emmanuel De Moor, Colorado School of Mines; Kishlay Mishra, Nucor Castrip Arkansas LLC; Lijia Zhao, ArcelorMittal Global R&D

**Monday PM | October 18, 2021**  
**A210 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**4:00 PM**

**High Strength Low Alloy Steels strengthened by Heusler precipitates:** Rafael Rodriguez De Vecchis<sup>1</sup>; Minal Shah<sup>1</sup>; Yuankang Wang<sup>1</sup>; Xin Wang<sup>1</sup>; Soumya Sridar<sup>1</sup>; Zhangwei Wang<sup>1</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**4:20 PM**

**Development of Fine Grained Steel for Cold Heading Application:** Deepan N<sup>1</sup>; Manjini Sambandam<sup>1</sup>; <sup>1</sup>JSW Steel Ltd, Salem Works

## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Metallic Coated Advanced Steels — Liquid Metal Embrittlement and Advances in Coating Production

**Sponsored by:** AIST: Metallurgy Processing Products and Applications Technology Committee, AIST: Galvanizing Technology Committee

**Program Organizers:** Joseph McDermid, McMaster University; Frank Goodwin, ILZRO

**Monday PM | October 18, 2021**  
**A211 | Greater Columbus Convention Center**

**Session Chairs:** Joseph McDermid, McMaster University; Frank Goodwin, International Zinc Association

#### 2:00 PM

**Influence of Temperature on the Mechanical Behavior of TRIP1180 Spot Welds with Liquid Metal Embrittlement Cracks:** *Kayla Molnar*<sup>1</sup>; Kip Findley<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Colorado School of Mines

#### 2:20 PM

**Liquid Metal Embrittlement in TRIP and Martensitic Ultrahigh Strength Steels:** *Pallavi Pant*<sup>1</sup>; Emmitt Fagerstrom<sup>1</sup>; Benjamin Hilpert<sup>2</sup>; Holger Schubert<sup>2</sup>; Luke Brewer<sup>1</sup>; <sup>1</sup>The University of Alabama; <sup>2</sup>Daimler AG

#### 2:40 PM

**Galvanizing Sheet Steel Under SHS Conditions for the Development of Steel Microstructures:** *Borys Sereda*<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Dmytro Kruglyak<sup>1</sup>; Irina Kruglyak<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

#### 3:00 PM

**A Study on Mechanical and Super-hydrophobic Behavior of the SiO<sub>2</sub>@ZnO Nano Core-shell Based Polymeric Coating:** *Jaya Verma*<sup>1</sup>; Deepak Kumar<sup>1</sup>; <sup>1</sup>IIT Delhi

#### 3:20 PM

**Use of the New Integrated Indicator ECP-Zn for Control Zinc Coating Obtaining Under SHS Conditions:** *Borys Sereda*<sup>1</sup>; *Dmytro Sereda*<sup>1</sup>; Irina Kruglyak<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

## ARTIFICIAL INTELLIGENCE

### AI for Big Data Problems in Advanced Imaging, Materials Modeling and Automated Synthesis — Artificial Intelligence for Automated Synthesis and Characterization

**Sponsored by:** TMS: Computational Materials Science and Engineering Committee

**Program Organizers:** Mathew Cherukara, Argonne National Lab; Badri Narayanan, University of Louisville; Subramanian Sankaranarayanan, University of Illinois (Chicago)

**Monday PM | October 18, 2021**  
**A124 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

#### 2:00 PM

**Improving EBM NIR Image Analysis for Component Qualification a Statistical Learning Approach:** *Michael Sprayberry*<sup>1</sup>; John Ledford<sup>1</sup>; Michael Kirka<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

#### 2:20 PM

**A Deep Generative Model for Parametric EBSD Pattern Simulation:** *Zihao Ding*<sup>1</sup>; Marc Graef<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

#### 2:40 PM Invited

**Non-iterative Deep Learning for High-fidelity Microscopic Tomography:** *Singanallur Venkatakrishnan*<sup>1</sup>; Amir Koushyar Ziabari<sup>1</sup>; Jacob Hinkle<sup>1</sup>; Micheal Kirka<sup>1</sup>; Jeffrey Warren<sup>1</sup>; Hassina Bilheux<sup>1</sup>; Vincent Paquit<sup>1</sup>; Ryan DeHoff<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

#### 3:00 PM

**Optimizing the Training of Convolutional Neural Networks for Image Segmentation:** *Benjamin Provencher*<sup>1</sup>; Aly Badran<sup>1</sup>; Jonathan Kroll<sup>1</sup>; Mike Marsh<sup>2</sup>; <sup>1</sup>University of Colorado; <sup>2</sup>Object Research Systems

#### 3:20 PM Break

#### 3:40 PM

**Semantic Segmentation of Porosity in In-situ X-ray Tomography Data Using FCNs:** *Pradyumna Elavarthi*<sup>1</sup>; Arun Bhattacharjee<sup>1</sup>; Anca Ralescu<sup>1</sup>; Ashley Paz y Puente<sup>1</sup>; <sup>1</sup>University of Cincinnati

#### 4:00 PM

**Machine-learning Based Algorithms for 4D X-ray Microtomographic Analysis:** *Hamidreza T-Sarraf*<sup>1</sup>; Sridhar Niverty<sup>1</sup>; Nikhilesh Chawla<sup>1</sup>; <sup>1</sup>Purdue University



# Technical Program

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## CERAMIC AND GLASS MATERIALS

### Ceramic Matrix Composites — Session II

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Narottam Bansal, NASA Glenn Research Center; Jacques Lamon, CNRS; Sung Choi, Naval Air Systems Command

**Monday PM | October 18, 2021**  
**B232 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**2:00 PM Invited**

**Ceramic Matrix Composite Technologies for Accident-tolerant Fuel Applications – Progress and Opportunities:** *Yutai Katoh*<sup>1</sup>; Takaaki Koyanagi<sup>1</sup>; David Arregui-Mena<sup>1</sup>; Peter Mouche<sup>1</sup>; Ken Kane<sup>1</sup>; Peng Xu<sup>2</sup>; Christian Deck<sup>3</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Idaho National Laboratory; <sup>3</sup>General Atomics

**2:40 PM**

**Synergistic Effects of Oxidation and Applied Load on SiC/BN/SiC Ceramic Matrix Composite Durability at Intermediate Temperatures:** Kaitlin Detwiler<sup>1</sup>; Marcus Dozer<sup>1</sup>; *Elizabeth Opila*<sup>1</sup>; <sup>1</sup>University of Virginia

**3:20 PM**

**Oxidation of BN Coatings in SiC/SiC Composites:** *Victoria Christensen*<sup>1</sup>; Frank Zok<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

**3:40 PM Break**

**4:00 PM**

**Development of Low Temperature, Dense Nano-composite Material Combining Electrophoretic and Atomic Layer Deposition Technique:** *Sumit Bhattacharya*<sup>1</sup>; Michael Pellin<sup>1</sup>; Abdellatif Yacout<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

**4:20 PM**

**High Temperature Composites Based on Zirconia Cement. High Temperature Composites Based on Ceramic Cements:** *Nickolai Iliukha*<sup>1</sup>; <sup>1</sup>Kyiv University

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Coatings to Protect Materials from Extreme Environments — Coatings and Surface Treatments for Extreme Environments

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Kang Lee, NASA Glenn Research Center; Yutaka Kagawa, The University of Tokyo; Daniel Mumm, University of California, Irvine; Rodney Trice, Purdue University; Emmanuel Boakye, UES Inc.; Valerie Wiesner, NASA Langley Research Center; Edward Gorzkowski, Naval Research Laboratory; Scooter Johnson, Naval Research Laboratory

**Monday PM | October 18, 2021**  
**A222 | Greater Columbus Convention Center**

**Session Chairs:** Daniel Mumm, University of California, Irvine; Edward Gorzkowski, Naval Research Laboratory

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**2:00 PM**

**Aerosol Deposition and Characterization of Sodium Niobate:** *Eric Patterson*<sup>1</sup>; Heonjune Ryou<sup>1</sup>; Edward Gorzkowski<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory

**2:30 PM**

**Functionally Graded Corrosion Resistant Coatings for Molten Salt Reactor Systems:** *Holly Garich*<sup>1</sup>; Tim Hall<sup>1</sup>; Stephen Raiman<sup>2</sup>; Bruce Pint<sup>3</sup>; <sup>1</sup>Faraday Technology; <sup>2</sup>Texas A&M University; <sup>3</sup>Oak Ridge National Laboratory

**2:50 PM**

**Effects of Laser Remediation Treatments on Global vs Local Environmentally-assisted Cracking of 5xxx Series Aluminum Alloy Ship Plate:** *Yang Liu*<sup>1</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University

**3:10 PM Break**

**3:30 PM**

**Electrodeposition of Functionally-graded Interlayers for Joining Plasma-facing Components and Heat-sinks for Nuclear Fusion Reactors:** *Katherine Lee*<sup>1</sup>; Brian Skinn<sup>1</sup>; Steve Snyder<sup>1</sup>; Maria Inman<sup>1</sup>; <sup>1</sup>Faraday Technology, Inc.

**3:50 PM**

**The Efficacy of Inorganic Zinc-Rich Primers to Mitigate Stress Corrosion Susceptibility in Al-Mg Alloys:** *Matthew McMahon*<sup>1</sup>; Allison Akman<sup>1</sup>; Eric Dau<sup>2</sup>; <sup>1</sup>Naval Surface Warfare Center, Carderock Division; <sup>2</sup>Vision Point Systems, LLC.

## NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — 1D Nanostructures

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**Monday PM | October 18, 2021**  
**B240/241 | Greater Columbus Convention Center**

**Session Chairs:** Haitao Zhang, University of North Carolina at Charlotte; Sanjay Mathur, University of Cologne

**2:00 PM Invited**

**Self-Assembled Periodic Nanostructures of SrSnO<sub>3</sub> Using Martensitic Phase Transformations:** *Bharat Jalan*<sup>1</sup>; <sup>1</sup>University of Minnesota

**2:40 PM**

**Growth Mechanism Study of Boron Carbide Nanowires:** *Manira Akter*<sup>1</sup>; Terry Xu<sup>1</sup>; <sup>1</sup>University of North Carolina Charlotte

**3:00 PM**

**Mechanism Study of Controlled Growth of Transition Metal Oxide Nanostructures:** *Haitao Zhang*<sup>1</sup>; <sup>1</sup>University of North Carolina at Charlotte

**3:20 PM Break**

**3:40 PM**

**NiO Nanostructure Growth at High Temperature in Water Vapor via In-situ ESEM:** *Boyi Qu*<sup>1</sup>; Klaus van Benthem<sup>1</sup>; <sup>1</sup>University of California Davis

**4:00 PM**

**Nanotube Consolidations and Metal-PTFE Nanocomposites for Conformable Thermal and Electrical Interfaces:** *Christopher Kovacs*<sup>1</sup>; Timothy Haugan<sup>2</sup>; Robert Ansel<sup>3</sup>; <sup>1</sup>Scintillating Solutions LLC; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>Linseis Inc.

**4:20 PM**

**Effect of Doping Carbon Nanotubes with Group III-V Compounds Using Floating Catalyst Method:** *Anuptha Pujari*<sup>1</sup>; Mark Schulz<sup>1</sup>; <sup>1</sup>Nanoworld Laboratories, University of Cincinnati

## SPECIAL TOPICS

### Curricular Innovations and Continuous Improvement of Academic Programs (and Satisfying ABET along the Way): The Elizabeth Judson Memorial Symposium — Course Innovations

**Sponsored by:** TMS: Accreditation Committee, TMS: Education Committee

**Program Organizers:** Alison Polasik, Campbell University; Susan Gentry, University of California, Davis; Jeffrey Fergus, Auburn University; Assel Aitkaliyeva, University of Florida; Kester Clarke, Colorado School of Mines; Subhadra Gupta, University of Alabama; Gregg Janowski, University of Alabama at Birmingham; M. Norton, Washington State University

**Monday PM | October 18, 2021**  
**B144/145 | Greater Columbus Convention Center**

**Session Chair:** Alison Polasik, Campbell University

**2:00 PM Introductory Comments**

**2:05 PM**

**Online Instruction of a Large Introductory Materials Course: A Partially Asynchronous Approach:** *Jonathan Brown*<sup>1</sup>; Jenifer Locke<sup>1</sup>; <sup>1</sup>The Ohio State University

**2:25 PM**

**Reframing Lab Courses to Improve Both Student Engagement and ABET Alignment:** *Timothy Chambers*<sup>1</sup>; <sup>1</sup>University of Michigan

**2:45 PM**

**Integrating Problem Based Learning into a Metals Processing Class:** *Peter Collins*<sup>1</sup>; <sup>1</sup>Iowa State University

**3:05 PM Break**

**3:20 PM Panel Discussion:** Discussion About the Future of Online Materials Education

## FUNDAMENTALS AND CHARACTERIZATION

### Deformation-induced Phase Transformations — Deformation-induced Phase Transformations

**Program Organizers:** Yangyang Zhao, Purdue University; Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Janelle Wharry, Purdue University

**Monday PM | October 18, 2021**  
**B132 | Greater Columbus Convention Center**

**2:00 PM Invited**

**Ausforming of Ferrium M54 Ultra-high Strength Steel:** *Suveen Mathaudhu*<sup>1</sup>; Yiwei Sun<sup>2</sup>; Joshua Edwards<sup>1</sup>; Jeffrey Lin<sup>3</sup>; Thomas Kozmel<sup>3</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Southeast University; <sup>3</sup>Questek Innovations, LLC

# Technical Program

## 2:40 PM

**Analysis of Stress State of Plastic Medium Influence on Structural Transformations in Low-alloy Steels:** Anton Matiukhin<sup>1</sup>; *Sergey Sheyko*<sup>2</sup>; Vldimir Tsyganov<sup>1</sup>; Valeriy Naumyk<sup>1</sup>; Anna Ben<sup>1</sup>; <sup>1</sup>"Zaporizhzhia Polytechnic" National University; <sup>2</sup>Zaporizhzhia National University

## 3:00 PM

**Localized Phase Transformation at Stacking Faults and the Corresponding Alloy Design Strategy:** *Longsheng Feng*<sup>1</sup>; Ashton Egan<sup>1</sup>; Timothy Smith<sup>2</sup>; Shakthipriya Baskar<sup>1</sup>; Michael Mills<sup>1</sup>; Maryam Ghazisaedi<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>NASA Glenn Research Center

## 3:20 PM Break

## 3:40 PM Invited

**Intrinsic Coupling between Deformation Twinning and Phase Transformation in NiTi Shape Memory Alloys and Metastable Beta Ti-alloys:** Yipeng Gao<sup>1</sup>; Qianglong Liang<sup>1</sup>; Yufeng Zheng<sup>1</sup>; Dong Wang<sup>2</sup>; Michael Mills<sup>1</sup>; Hamish Fraser<sup>1</sup>; *Yunzhi Wang*<sup>1</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Xian Jiao Tong University

## 4:20 PM

**Solid Phase Plasticity Mechanisms in Metals and Rocks during Shear Deformation:** *Suveen Mathaudhu*<sup>1</sup>; Arun Devaraj<sup>2</sup>; <sup>1</sup>Colorado School of Mines / Pacific Northwest National Laboratory; <sup>2</sup>Pacific Northwest National Laboratory

## 4:40 PM

**Accounting for Phase Transformation in Plastic Anisotropy Modeling of SS316L:** Elizabeth Mamros<sup>1</sup>; Jinjin Ha<sup>1</sup>; *Yannis Korkolis*<sup>2</sup>; Brad Kinsey<sup>1</sup>; <sup>1</sup>University of New Hampshire; <sup>2</sup>Ohio State University

## PROCESSING AND MANUFACTURING

### Development of Light Weight Alloys and Composites — Microstructure and Processing: Composites II

**Program Organizers:** Ramasis Goswami, Naval Research Laboratory; Nikhil Gupta, New York University; Tanjore Jayaraman, University of Michigan-Dearborn; Aashish Rohatgi, Pacific Northwest National Laboratory

## Monday PM | October 18, 2021

A214 | Greater Columbus Convention Center

**Session Chairs:** Nikhil Gupta, New York University, Tandon School of Engineering; Tanjore Jayaraman, College of Engineering and Computer Science, University of Michigan-Dearborn

## 2:00 PM Invited

**Impact of Laser Shock Peening on Stress Corrosion Susceptibility in Al-Mg Alloys:** *Eric Dau*<sup>1</sup>; William Golumbskie<sup>2</sup>; Matthew McMahon<sup>2</sup>; <sup>1</sup>Vision Point Systems, LLC.; <sup>2</sup>Naval Surface Warfare Center, Carderock Division

## 2:40 PM Invited

**Low Cycle Fatigue Behavior of Conventional High Temperature Titanium Alloys for Aeroengine Applications:** *Ramachandra Canumalla*<sup>1</sup>; <sup>1</sup>Vice President and Chief Technology Officer

## 3:20 PM

**Investigation of Microstructure, Interfaces and Mechanical Properties of Metal Matrix Composites:** *Ramasis Goswami*<sup>1</sup>; <sup>1</sup>Naval Research Laboratory

## 3:40 PM Break

## 4:00 PM

**Magnesium Alloy Composite with Metal Reinforced Particles Using Friction Stir Processing To Improve Mechanical Properties:** *Sangam Sangral*<sup>1</sup>; Jayaprakash Murugesan<sup>1</sup>; Mahesh Patel<sup>1</sup>; Achyuth Kulkarni<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Indore

## 4:20 PM

**Inoculation of ML5 Cast Magnesium Alloy with Carbon Nano Powder:** *Spartak Makovskyi*<sup>1</sup>; Vadym Shalomeev<sup>2</sup>; Volodymir Klochykhin<sup>1</sup>; <sup>1</sup>Motor Sich JSC; <sup>2</sup>National University Zaporozhye Polytechnica

## 4:40 PM

**Insights into Metal-based Polymer Pyrolysis for In-situ MMC Production:** *Aaron Gladstein*<sup>1</sup>; Alan Taub<sup>1</sup>; <sup>1</sup>University of Michigan

## ENERGY

### Energy Materials for Sustainable Development — Solar Energy Conversion

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

## Monday PM | October 18, 2021

A216 | Greater Columbus Convention Center

**Session Chairs:** Scott Mixture, Alfred University; Kenneth Sandhage, Purdue University

## 4:00 PM

**The Role of Amorphous TiO<sub>2</sub> Film in Performance of Si Photoanodes for Hydrogen Production by Photoelectrochemical Water Splitting:** *Mehrdad Abbasi Gharacheh*<sup>1</sup>; Jun Meng<sup>2</sup>; Yutao Dong<sup>2</sup>; Dane Morgan<sup>2</sup>; Xudong Wang<sup>2</sup>; Jinwoo Hwang<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>University of Wisconsin-Madison

## 4:20 PM Invited

**New Types of Oxides, Chalcogenide and Phosphide Catalyst for Water Splitting:** *Daniel Chua*<sup>1</sup>; <sup>1</sup>National University of Singapore

## 4:50 PM Invited

**Engineering Nanoscale Semiconductor-catalyst Interfaces for Low-cost Carbon-free Technology:** *Flavio de Souza*<sup>1</sup>; <sup>1</sup>Brazilian Center for Research in Energy and Materials

## CERAMIC AND GLASS MATERIALS

### Glasses and Optical Materials: Current Issues and Functional Applications — Optical Properties and Processing of Amorphous Solids

**Sponsored by:** ACerS Basic Science Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Delia Brauer, Otto Schott Institute of Materials Research

**Monday PM | October 18, 2021**  
**B231 | Greater Columbus Convention Center**

**Session Chair:** Jungmin Ha, Lawrence Livermore National Laboratory

**2:00 PM**

**3D Printed Germania-titania-silica Glasses to Tune the Refractive Index and Abbe Number:** *Jungmin Ha*<sup>1</sup>; Koroush Sasan<sup>1</sup>; Timothy Yee<sup>2</sup>; Andrew Lange<sup>3</sup>; Du Nguyen<sup>1</sup>; Nikola Dudukovic<sup>1</sup>; Oscar Herrera<sup>1</sup>; Christopher Mah<sup>1</sup>; Rebecca Dylla-Spears<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

**2:20 PM**

**Local Structural Effects on Divalent Europium in Glass Host Materials:** *Charles Bellows*<sup>1</sup>; <sup>1</sup>Alfred University

**2:40 PM**

**Optical Properties of One-dimensional Nb2O5 Nanostructures Prepared by Electrospinning:** *Tomasz Tanski*<sup>1</sup>; Weronika Smok<sup>1</sup>; Marta Zaborowska<sup>1</sup>; <sup>1</sup>Silesian University of Technology

## FUNDAMENTALS AND CHARACTERIZATION

### Grain Boundaries, Interfaces, and Surfaces in Ceramics: Fundamental Structure—Property—Performance Relationships — Continuum Approaches

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Rheinheimer Wolfgang, Forschungszentrum Jülich; Catherine Bishop, University of Canterbury; Shen Dillon, University of California, Irvine; Ming Tang, Rice University; John Blendell, Purdue University; Wayne Kaplan, Technion - Israel Institute of Technology; Melissa Santala, Oregon State University

**Monday PM | October 18, 2021**  
**B244/245 | Greater Columbus Convention Center**

**Session Chairs:** Wolfgang Rheinheimer, Forschungszentrum Jülich; John Blendell, Purdue University

**2:00 PM Invited**

**Microstructure-within-a-microstructure: Understanding Critical Structural Variations within Grain Boundary Networks:** *Timothy Rupert*<sup>1</sup>; <sup>1</sup>University of California, Irvine

**2:40 PM Invited**

**Elucidating Grain Boundary Motion with 4D Grain Growth Measurements Using Non-destructive X-ray Diffraction Grain Mapping:** *Amanda Krause*<sup>1</sup>; <sup>1</sup>University of Florida

**3:20 PM Break**

**3:40 PM**

**Effect of Sodium on the Processability and Mechanical Properties of Nanocrystalline**

**Magnesium Aluminate:** *Isabella Loureiro Muller Costa*<sup>1</sup>; Ricardo Castro<sup>1</sup>; Joice Miagava<sup>2</sup>; <sup>1</sup>University of California Davis; <sup>2</sup>Insper – Institute of Education and Research

## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Materials Discovery and Design II

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Monday PM | October 18, 2021**  
**B131 | Greater Columbus Convention Center**

**Session Chairs:** Dan Thoma, University of Wisconsin-Madison; Keith Knipling, Naval Research Laboratory

**2:00 PM Invited**

**Compositionally Complex Oxides: Synthesis, Characterization, Challenges, and Opportunities:** *Veerle Keppens*<sup>1</sup>; <sup>1</sup>University of Tennessee

**2:30 PM Invited**

**High-throughput Design and Processing of MPEAs Using Additive Manufacturing:** *Dan Thoma*<sup>1</sup>; Michael Niezgoda<sup>1</sup>; Phalgun Nelaturu<sup>1</sup>; Zahabul Islam<sup>1</sup>; Michael Moorehead<sup>1</sup>; Adrien Couet<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**2:50 PM Invited**

**Refractory High Entropy Alloys with Balanced Properties Tailored for Service Conditions:** *Andrew Detor*<sup>1</sup>; Scott Oppenheimer<sup>1</sup>; James Ruud<sup>1</sup>; Emily Cheng<sup>1</sup>; <sup>1</sup>GE Research

**3:10 PM Invited**

**Microstructures of Al<sub>2.7</sub>CrFeMnV, Al<sub>2.7</sub>CrFeTiV, and Al<sub>2.7</sub>CrMnTiV High-entropy Alloys:** *Patrick Callahan*<sup>1</sup>; Keith Knipling<sup>1</sup>; <sup>1</sup>Naval Research Laboratory



# Technical Program

## 3:30 PM Break

### 3:50 PM

**Design of TWIP/TRIP Non-equimolar High-entropy Alloys:** *Xin Wang*<sup>1</sup>; Rafael Tomás Rodríguez De Vecchis<sup>2</sup>; Chenyang Li<sup>3</sup>; Wei Chen<sup>3</sup>; Wei Xiong<sup>2</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Physical Metallurgy and Materials Design Laboratory, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, PA, 15261, USA; <sup>3</sup>Department of Mechanical, Materials and Aerospace Engineering, Illinois Institute of Technology, Chicago, IL, 60616 USA

### 4:10 PM

**Nanostructured Oxide-dispersion-strengthened CoCrFeMnNi High-entropy Alloys:** Xiang Zhang<sup>1</sup>; *Fei Wang*<sup>1</sup>; Xing-Zhong Li<sup>1</sup>; Khalid Hattar<sup>2</sup>; Bai Cui<sup>1</sup>; <sup>1</sup>University of Nebraska-Lincoln; <sup>2</sup>Sandia National Laboratories

### 4:30 PM Invited

**Exploring the Feasible High Entropy Alloy Space:** *Raymundo Arroyave*<sup>1</sup>; <sup>1</sup>Texas A&M University

### 4:50 PM

**Development of Low-cost High Entropy Alloys through Alloy Mixing:** *Karthikeyan Hariharan*<sup>1</sup>; Katakam Sivaprasad<sup>1</sup>; <sup>1</sup>National Institute of Technology, Tiruchirappalli

## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III — Session II

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**Monday PM | October 18, 2021**

**B246 | Greater Columbus Convention Center**

**Session Chairs:** M Arul Kumar, Los Alamos National Laboratory; Aaron Tallman, Los Alamos National Laboratory

### 2:00 PM Invited

**Developing Surrogate Models for Crystal Plasticity-based Creep by Leveraging Macroscale Constitutive Relations:** *Aaron Tallman*<sup>1</sup>; Laurent Capolungo<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratories

### 2:30 PM

**Weldment Finite Element Modeling and Validation for Integration with CALPHAD Tools:** *Daniel Bechetti*<sup>1</sup>; Jacob Steiner<sup>1</sup>; Charles Fisher<sup>1</sup>; <sup>1</sup>Naval Surface Warfare Center, Carderock Division

### 2:50 PM

**Rapid Screening of High-throughput Ground State Predictions:** *Sayan Samanta*<sup>1</sup>; Axel van de Walle<sup>1</sup>; <sup>1</sup>Brown University

### 3:10 PM Invited

**Lab-based Diffraction Contrast Tomography: Achieving Large Volume Grain Statistics for Full Field Modeling of Polycrystalline Materials:** Jun Sun<sup>1</sup>; Jette Oddershede<sup>1</sup>; Florian Bachmann<sup>1</sup>; Hrshikesh Bale<sup>2</sup>; *William Harris*<sup>3</sup>; Erik Lauridsen<sup>1</sup>; <sup>1</sup>Xnovo Technology; <sup>2</sup>Carl Zeiss X-ray Microscopy; <sup>3</sup>Carl Zeiss Microscopy, LLC

## 3:50 PM Break

### 4:10 PM

**Physics-based Full-Field Fast Fourier Transform Modeling of Creep Behavior: Application to 347H Steel:** *Mariyappan Arul Kumar*<sup>1</sup>; Ricardo Lebensohn<sup>1</sup>; Laurent Capolungo<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

### 4:30 PM

**A Physics-based Crystal Plasticity Constitutive Model Incorporating the Dynamic Strain Aging: Application to 347H Steel:** *Veerappan Prithvirajan*<sup>1</sup>; Nathan Beets<sup>1</sup>; M Arul Kumar<sup>1</sup>; Bjorn Clausen<sup>1</sup>; Ricardo Lebensohn<sup>1</sup>; Laurent Capolungo<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

### 4:50 PM

**Full-field Modeling of Vacancy Diffusion in a Crystal Plasticity Framework:** *Aritra Chakraborty*<sup>1</sup>; Nathan Beets<sup>1</sup>; Mariyappan Arul Kumar<sup>1</sup>; Ricardo Lebensohn<sup>1</sup>; Laurent Capolungo<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

### 5:10 PM

**Simulation of Creep and Uniaxial Strain in 316H Steel via a Fully Mechanistic Fast Fourier Transform Based Crystal Plasticity Constitutive Model:** *Nathan Beets*<sup>1</sup>; Laurent Capolungo<sup>1</sup>; Mariyappan Arul Kumar<sup>1</sup>; Ricardo Lebensohn<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

## PROCESSING AND MANUFACTURING

### Light Metal Technology — Forming Technology

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Xiaoming Wang, Purdue University; Yufeng Zheng, University of Nevada-Reno

**Monday PM | October 18, 2021**

**A213 | Greater Columbus Convention Center**

**Session Chair:** Tao Wang, Rio Tinto

### 2:00 PM

**Effect of Vacuum Level on Porosity and Mechanical Properties of Aluminum Alloys in High-pressure Die Casting:** *Nicole Trometer*<sup>1</sup>; Emre Cinkilic<sup>1</sup>; Larry Godlewski<sup>2</sup>; Eben Prabhu<sup>2</sup>; Alan Luo<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Ford Motor Company

### 2:20 PM

**Lattice Site Correspondence and Morphology of Al<sub>6</sub>Mn Precipitate:** *Yuchi Wang*<sup>1</sup>; Yunzhi Wang<sup>1</sup>; Daniel Freiberg<sup>2</sup>; Yang Huo<sup>2</sup>; Wendi Zhu<sup>2</sup>; Robert Williams<sup>1</sup>; Mei Li<sup>2</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Ford

### 2:40 PM

**Comparison of Acoustic Softening Phenomenon in Tensile Tests and Incremental Sheet Forming:** *Randy Cheng*<sup>1</sup>; Jiarui Kang<sup>2</sup>; Xun Liu<sup>2</sup>; Alan Taub<sup>1</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>The Ohio State University

### 3:00 PM

**START: Rio Tinto's 'Nutrition Label' for Sustainable Aluminium:** *Tao Wang*<sup>1</sup>; <sup>1</sup>Rio Tinto

## CERAMIC AND GLASS MATERIALS

### Manufacturing and Processing of Advanced Ceramic Materials — New Opportunities in Ceramic Processing II

**Sponsored by:** ACerS Manufacturing Division

**Program Organizers:** Bai Cui, University of Nebraska-Lincoln; James Hemrick, Oak Ridge National Laboratory; Mike Alexander, Allied Mineral Products; Eric Faierman, Quad City Manufacturing Laboratory/Western Illinois University; Keith DeCarlo, Blasch Precision Ceramics

**Monday PM | October 18, 2021**  
**B234 | Greater Columbus Convention Center**

**Session Chairs:** Ivar Reimanis, Colorado School of Mines; Jian Luo, University of California, San Diego

#### 2:00 PM Invited

**Flash Sintering, Ultrafast Sintering without Electric Fields, and Electric Field Effects on Microstructural Evolution:** *Jian Luo*<sup>1</sup>; <sup>1</sup>University of California, San Diego

#### 2:40 PM Invited

**High Temperature Coatings for Concentrated Solar Power Receivers:** Julia Billman<sup>1</sup>; Ivar Reimanis<sup>1</sup>; Andrea Ambrosini<sup>2</sup>; Gregory Jackson<sup>1</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Sandia National Laboratory

#### 3:20 PM

**Green State Joining of Silicon Carbide for High-temperature Applications:** Olivia Brandt<sup>1</sup>; Rodrigo Orta Guerra<sup>1</sup>; Rodney Trice<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; <sup>1</sup>Purdue University

#### 3:40 PM Break

#### 4:00 PM

**Self-propagating High Temperature Synthesis of Chevrel Phase Compounds:** Milind Pawar<sup>1</sup>; <sup>1</sup>The Ohio State University

## CERAMIC AND GLASS MATERIALS

### Phase Transformations in Ceramics: Science and Applications — Experimental Studies on Structure and Control II

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Scott McCormack, University of California, Davis; Pankaj Sarin, Oklahoma State University; Sanjay V. Khare, University of Toledo; Waltraud Kriven, University of Illinois at Urbana-Champaign

**Monday PM | October 18, 2021**  
**B230 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

#### 2:00 PM Invited

**Symmetry-mode Analysis of Phase Transitions in Solids:** Branton Campbell<sup>1</sup>; Harold Stokes<sup>2</sup>; <sup>1</sup>Brigham Young University; <sup>2</sup>Brigham Young Univ

#### 2:30 PM Invited

**High Pressure Phase Transformations of Zircon-type Silicate Materials:** Xiaofeng Guo<sup>1</sup>; Andrew Strzelecki<sup>1</sup>; Xiaodong Zhao<sup>1</sup>; Jason Baker<sup>2</sup>; Stella Chariton<sup>3</sup>; Vitali Prakapenka<sup>3</sup>; Hongwu Xu<sup>4</sup>; <sup>1</sup>Washington State University; <sup>2</sup>Lawrence Livermore National Laboratory; <sup>3</sup>The University of Chicago; <sup>4</sup>Los Alamos National Laboratory

#### 3:00 PM Invited

**Initial Stages of Transformation of 2-D Assemblies of Nanosheets to Tunnel Structures:** Scott Misture<sup>1</sup>; <sup>1</sup>Alfred University

#### 3:30 PM Break

#### 3:50 PM

**Crystallographic Studies of the Leucite-pollucite System Synthesized by Geopolymer Crystallization:** Andrew Steveson<sup>1</sup>; Waltraud Kriven<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

#### 4:10 PM

**In-situ Phase Equilibria in the TiO<sub>2</sub>-HfO<sub>2</sub>-WO<sub>3</sub> System up to 1400°C:** Benjamin Hulbert<sup>1</sup>; Dylan Blake<sup>1</sup>; Waltraud Kriven<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

## FUNDAMENTALS AND CHARACTERIZATION

### Probing Defect Properties and Behavior under Mechanical Deformation and Extreme Conditions — In Situ and Advanced Characterization of Defects

**Sponsored by:** TMS Nanomechanical Materials Behavior Committee, TMS Nuclear Materials Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Zhe Fan, Lamar University; Tianyi Chen, Oregon State University; Shijun Zhao, City University of Hong Kong; Mitra Taheri, Johns Hopkins University; Yuri Osetskiy, Oak Ridge National Laboratory

**Monday PM | October 18, 2021**  
**B140/141 | Greater Columbus Convention Center**

**Session Chairs:** Xiaoqing Pan, University of California Irvine; Xinghang Zhang, Purdue University

#### 2:00 PM Invited

**Imaging Electronic Properties of Ferroelectric Interfaces and Domain Walls via 4D STEM:** Christopher Addiego<sup>1</sup>; Huaixun Huyan<sup>1</sup>; Xiaoqing Pan<sup>1</sup>; <sup>1</sup>University of California Irvine

#### 2:30 PM Invited

**Ultra-high Strength and Plasticity Mediated by Partial Dislocations and Defect Networks:** Ruizhe Su<sup>1</sup>; Dajla Neffati<sup>2</sup>; Yashashree Kulkarni<sup>2</sup>; Xinghang Zhang<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>University of Houston

#### 3:00 PM

**Probing Materials Properties across Scales with Scanning Diffraction in Transmission Electron Microscopy:** Wenpei Gao<sup>1</sup>; <sup>1</sup>North Carolina State University

#### 3:20 PM Break

#### 3:40 PM

**In-situ Study of Failure Defects in Cu/Nb Nanolaminates under Deformation:** Yifan Zhang<sup>1</sup>; Nan Li<sup>1</sup>; Laurent Capolungo<sup>1</sup>; Matt Schneider<sup>1</sup>; Rodney McCabe<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

# Technical Program

## 4:00 PM Invited

**In-situ Transmission Electron Microscopy of Intermittent Dislocation Activities and Deformation Mechanisms:** *Jian Min Zuo*<sup>1</sup>; Haw-Wen Hsiao<sup>1</sup>; Yang Hu<sup>1</sup>; Qun Yang<sup>1</sup>; <sup>1</sup>University of Illinois

## 4:30 PM

**The Effects of Sample-preparation-induced Defects on the Mechanical Properties of Single Crystal Aluminum Nano-pillars:** *Yang Yang*<sup>1</sup>; Sarah Wang<sup>2</sup>; Bin Xiang<sup>3</sup>; Sheng Yin<sup>2</sup>; Thomas Pekin<sup>2</sup>; Xiaoqing Li<sup>2</sup>; Ruopeng Zhang<sup>2</sup>; Kayla Yano<sup>4</sup>; David Hwang<sup>5</sup>; Mark Asta<sup>1</sup>; Costas Grigoropoulos<sup>2</sup>; Frances Allen<sup>1</sup>; Andrew Minor<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory; <sup>2</sup>UC Berkeley; <sup>3</sup>USTC; <sup>4</sup>PNPL; <sup>5</sup>Stony Brook University

## 4:50 PM

**In-situ Studies on Radiation Response of a Nanotwinned Steel:** *Zhongxia Shang*<sup>1</sup>; Tongjun Niu<sup>1</sup>; Tianyi Sun<sup>1</sup>; Sichuang Xue<sup>1</sup>; Wei-Ying Chen<sup>2</sup>; Meimei Li<sup>2</sup>; Haiyan Wang<sup>1</sup>; Xinghang Zhang<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Argonne National Laboratory

## SPECIAL TOPICS

### Research Lightning Talks — Research Lightning Talks I

**Sponsored by:** ACerS President's Council of Student Advisors

**Program Organizers:** Victoria Christensen, University of California Santa Barbara; Michael Walden, Colorado School of Mines; Erin Louise Valenzuela, University of Birmingham; Katelyn Kirchner, Pennsylvania State University; Andrew Ericks, University of California, Santa Barbara

**Monday PM | October 18, 2021**

**B142/143 | Greater Columbus Convention Center**

**Session Chairs:** Tess Marconie, Purdue University; Averyonna Kimery, Purdue University

## 2:00 PM Introductory Comments

## 2:10 PM

**Will Low-cost Ceramic Water Filters Really Work?:** *Ian Nettleship*<sup>1</sup>; <sup>1</sup>University of Pittsburgh

## 2:15 PM

**Refractories for the Food Industry:** *Ryan Hershey*<sup>1</sup>; <sup>1</sup>Allied Mineral Products, Inc.

## 2:20 PM

**Using Unsupervised Learning to Understand Thin Film Growth:** *Kimberly Gliebe*<sup>1</sup>; Alp Sehrioglu<sup>1</sup>; <sup>1</sup>Case Western Reserve University

## 2:25 PM

**Direct Ink Writing with Highly Loaded Aqueous Silicon Carbide Suspensions:** *Tess Marconie*<sup>1</sup>; Kyle Cox<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; Rodney Trice<sup>1</sup>; <sup>1</sup>Purdue University

## 2:30 PM

**Germanium Photodiodes for Capture of High Energy X-rays:** *Joseph Wood*<sup>1</sup>; Klaus van Benthem<sup>1</sup>; Charles Hunt<sup>1</sup>; <sup>1</sup>University of California, Davis

## 2:35 PM

**Joining of Silicon Carbide for High-temperature Applications:** *Olivia Brandt*<sup>1</sup>; Rodrigo Orta Guerra<sup>1</sup>; Rodney Trice<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; <sup>1</sup>Purdue University

## 2:40 PM

**Mechanical behavior of bonded-PDMS for biological payloads in microgravity:** *Annaliza Perez-Torres*<sup>1</sup>; <sup>1</sup>Space Tango

## 2:45 PM

**Perfecting Steel Processing in the 21st Century:** *Alyssa Stubbers*<sup>1</sup>; Thomas Balk<sup>1</sup>; <sup>1</sup>University of Kentucky

## 2:50 PM

**Superalloy Development for Specific Applications: A Low CTE Alloy:** *Thomas Mann*<sup>1</sup>; <sup>1</sup>Purdue University

## MATERIALS-ENVIRONMENT INTERACTIONS

### Thermodynamics of Materials in Extreme Environments — Thermodynamics and Stabilities of Alloys and Ceramics

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division

**Program Organizers:** Xiaofeng Guo, Washington State University; Kristina Lilova, Arizona State University; Kyle Brinkman, Clemson University; Alexandra Navrotsky, Arizona State University; Jake Amoroso, Savannah River National Laboratory; Xingbo Liu, West Virginia University; Gustavo Costa, NASA Glenn Research Center

**Monday PM | October 18, 2021**

**A221 | Greater Columbus Convention Center**

**Session Chairs:** Kristina Lilova, Arizona State University; Xiaofeng Guo, Washington State University

## 4:00 PM Invited

**Stability of Multicomponent Rare Earth Silicates for Environmental Barrier Coating Application:** *Mackenzie Ridley*<sup>1</sup>; Cameron Miller<sup>1</sup>; Rebekah Webster<sup>1</sup>; Hans Olson<sup>1</sup>; Alejandro Salanova<sup>1</sup>; Kathleen Tomko<sup>1</sup>; Jon Ihlefeld<sup>1</sup>; Cormac Toher<sup>2</sup>; Patrick Hopkins<sup>1</sup>; *Elizabeth Opila*<sup>1</sup>; <sup>1</sup>University of Virginia; <sup>2</sup>Duke University

## 4:30 PM Invited

**Directions of Zero Thermal Expansion in Anisotropic Oxides:** *Scott McCormack*<sup>1</sup>; William Wheeler<sup>2</sup>; Benjamin Hulbert<sup>2</sup>; Waltraud Kriven<sup>2</sup>; <sup>1</sup>University of California, Davis; <sup>2</sup>University of Illinois at Urbana-Champaign

## 5:00 PM

**A First-principles-based Study of Oxidation Thermodynamics in Refractory High Entropy Alloys:** *Adib Samin*<sup>1</sup>; <sup>1</sup>Air Force Institute of Technology

## SPECIAL TOPICS

### MS&T21 Plenary Session — MS&T21 Plenary Session

Tuesday AM | October 19, 2021  
 Union Station Ballroom | Greater Columbus Convention Center

8:00 AM Welcome Comments

8:05 AM Introductory Comments

8:10 AM Plenary

AIST Adolf Martens Memorial Steel Lecture: Iron: The Ubiquitous Element: *Anil Sachdev*<sup>1</sup>; <sup>1</sup>General Motors Global Research and Development

8:50 AM Award Presentation

8:55 AM Introductory Comments

9:00 AM Plenary

TMS Institute of Metals/Robert Franklin Mehl Award for MS&T21: New Superalloys in the Co-Ni Design Space for 3D Printing: *Tresa Pollock*<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

9:40 AM Award Presentation

9:45 AM Introductory Comments

9:50 AM Plenary

ACerS Edward Orton, Jr. Memorial Lecture: Turning Down the Heat in Sintering to Enable the Unification of all Materials: *Clive Randall*<sup>1</sup>; <sup>1</sup>Pennsylvania State University

10:30 AM Award Presentation

10:35 AM Concluding Comments

## PROCESSING AND MANUFACTURING

### 13th Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing — Novel Approaches to Sustainable Manufacturing II

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Surojit Gupta, University of North Dakota; Rajiv Asthana, University of Wisconsin; Hisayuki Suematsu, Nagaoka University of Technology; Mritunjay Singh, Ohio Aerospace Institute; Enrico Bernardo, University of Padova; Yiquan Wu, Alfred University; Zhengyi Fu, Wuhan University of Technology; Allen Applett, Oklahoma State University; Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology

Tuesday PM | October 19, 2021  
 A212 | Greater Columbus Convention Center

**Session Chair:** Surojit Gupta, University of North Dakota

2:00 PM

A Comparative Study of Vibration Signatures of FDM 3D Printers under Different States of Operation: *Roshan Mishra*<sup>1</sup>; Kunal Kate<sup>1</sup>; <sup>1</sup>University of Louisville

2:20 PM

A Sustainable and Energy-efficient Electrochemical Technology for Dewatering of Cellulosic Nanomaterials: *Huong Le*<sup>1</sup>; Santosh Vijapur<sup>1</sup>; Timothy D. Hall<sup>1</sup>; E. Jennings Taylor<sup>1</sup>; Maria Inman<sup>1</sup>; Stephen Snyder<sup>1</sup>; Kim Nelson<sup>2</sup>; <sup>1</sup>Faraday Technology; <sup>2</sup>AVAPCO LLC

2:40 PM

Low-cost Ceramic Composite Membranes for Ultrafiltration of Produced Water: *Christine Watson*<sup>1</sup>; Pankaj Sarin<sup>1</sup>; V. V. Rohit Bukka<sup>1</sup>; <sup>1</sup>Oklahoma State University

## ARTIFICIAL INTELLIGENCE

### Accelerating Materials Science with Big Data and Machine Learning — Session II

**Program Organizers:** Huan Tran, Georgia Institute of Technology; Muratahan Aykol, Toyota Research Institute

Tuesday PM | October 19, 2021  
 A123 | Greater Columbus Convention Center

**Session Chair:** Christopher Kuenneth, Georgia Institute of Technology

2:00 PM Invited

Data Science as Bridge – Materials Characterization and Modeling: *Maria Chan*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

2:40 PM

Learning Synthesis: Engineering Metal Nanoclusters for Specific Material Properties: *Ryan McCarty*<sup>1</sup>; <sup>1</sup>University of California Irvine

3:00 PM

Characterization of Microscopic Deformation of Materials Using Deep Learning Methods: *Kavindu Wijesinghe*<sup>1</sup>; Janith Wann<sup>1</sup>; Natasha Banerjee<sup>1</sup>; Sean Banerjee<sup>1</sup>; Ajit Achuthan<sup>1</sup>; <sup>1</sup>Clarkson University

3:20 PM

A Data-driven Simulator for High-throughput Prediction of Electromigration-mediated Damage in Polycrystalline Interconnects: *Peichen Wu*<sup>1</sup>; William Farmer<sup>1</sup>; Kumar Ankit<sup>1</sup>; <sup>1</sup>Arizona State University

## SPECIAL TOPICS

### ACerS Frontiers of Science and Society: The Rustum Roy Lecture

**Sponsored by:** ACerS

Tuesday PM | October 19, 2021  
 B130 | Greater Columbus Convention Center

1:00 PM Invited

Advanced Ceramics for Energy and Environmental Technology: *Alexander Michaelis*<sup>1</sup>; <sup>1</sup>Fraunhofer Institute for Ceramic Technologies & Systems IKTS



# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — AM Modeling - Machine Learning and Artificial Intelligence

**Sponsored by:** TMS Computational Materials Science and Engineering Committee

**Program Organizers:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

**Tuesday PM | October 19, 2021**  
**A113 | Greater Columbus Convention Center**

**Session Chairs:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, CCDC Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeon-Gil Jung, Changwon National University

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**2:00 PM**  
**Deep Reinforcement Learning for Defect Mitigation in Laser Powder Bed Fusion**

: *Francis Ogoke*<sup>1</sup>; Amir Barati Farimani<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**2:20 PM**  
**Online Characterization of Melt Pool Dimensions Using Acoustic Monitoring and Deep Learning:** *Evan Diewald*<sup>1</sup>; Christian Gobert<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**2:40 PM**  
**Machine Learning – Assisted Navigation in the Additive Manufacturing Design Space:** *Maheer Alghalayini*<sup>1</sup>; Surya Kalidindi<sup>2</sup>; Chris Paredis<sup>1</sup>; Fadi Abdeljawad<sup>1</sup>; <sup>1</sup>Clemson University; <sup>2</sup>Georgia Institute of Technology

**3:00 PM**  
**Process Consistency in Laser Powder Bed Fusion Observed Through Large Scale Single Bead Melt Pool Measurements:** *Christian Gobert*<sup>1</sup>; Evan Diewald<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**3:20 PM**  
**Melt Pool Scale Modeling of Austenitic Stainless Steel Solidification Features in Laser Powder Bed Fusion:** *Joseph Aroh*<sup>1</sup>; P. Chris Pistorius<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**3:40 PM**  
**Gas Adsorption Analysis in 3D Printed Metal Organic Frameworks:** *Tejesh Dube*<sup>1</sup>; Hye-Yeong Park<sup>2</sup>; Yeon-Gil Jung<sup>2</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis; <sup>2</sup>Changwon National University

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Ceramic-based Materials: Process Development, Materials, Process Optimization and Applications — Session III: Laser Powder Bed Fusion and Novel AM Processes

**Sponsored by:** ACerS Engineering Ceramics Division, ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Xuan Song, University of Iowa; Lei Chen, University of Michigan-Dearborn; Xiangyang Dong, Missouri University of Science and Technology; Yiquan Wu, Alfred University; Paolo Colombo, University of Padova; Rajendra Bordia, Clemson University; Long-Qing Chen, Pennsylvania State University

**Tuesday PM | October 19, 2021**  
**A112 | Greater Columbus Convention Center**

**Session Chair:** Fei Peng, Clemson University

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**2:00 PM Invited**  
**Machine-learning-based Microstructure-property Prediction Enabled by High-throughput Ceramic Sample-array Preparation Using Integrated Additive/Subtractive Manufacturing:** Xiao Geng<sup>1</sup>; Jianan Tang<sup>1</sup>; Dongsheng Li<sup>2</sup>; Yunfeng Shi<sup>3</sup>; Rajendra Bordia<sup>4</sup>; Jianhua Tong<sup>1</sup>; Xiao Hai<sup>1</sup>; *Fei Peng*<sup>1</sup>; <sup>1</sup>Clemson University; <sup>2</sup>Advanced Manufacturing LLC; <sup>3</sup>Rensselaer Polytechnic Institute

**2:30 PM**  
**Direct-Ink-Writing and Cold-Sintering of ZnO Ceramics:** *Russell Maier*<sup>1</sup>; Igor Levin<sup>1</sup>; Lawrence Friedman<sup>1</sup>; Andrew Allen<sup>1</sup>; Abhay Goyal<sup>1</sup>; Nicos Martys<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**2:50 PM**  
**Additively Manufactured Carbon/Carbon Composites via Direct Ink Writing of Phenolic Resin Precursors:** *Caitlyn Clarkson*<sup>1</sup>; Connor Wyckoff<sup>1</sup>; William Costakis<sup>1</sup>; Matthew Dickerson<sup>1</sup>; Hilmar Koerner<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory

**3:10 PM**  
**Bulk Ferroelectric Metamaterial with Giant Piezoelectric Coefficients and Biomimetic Mechanical Property from Additive Manufacturing:** *Jun Li*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

## ADDITIVE MANUFACTURING

### Additive Manufacturing of High and Ultra-High Temperature Ceramics and Composites: Processing, Characterization and Testing — Laser-based Additive Manufacturing, New Methods, and Testing

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Corson Cramer, Oak Ridge National Laboratory; Greg Hilmas, Missouri University of Science and Technology; Lisa Rueschhoff, Air Force Research Laboratory

**Tuesday PM | October 19, 2021**

**A111 | Greater Columbus Convention Center**

**Session Chair:** Lisa Rueschhoff, Air Force Research Laboratory

**2:00 PM Invited**

**Additive Slurry Drying as a Novel Method for Realizing Large Ceramic Components Using AM:** Johannes Homa<sup>1</sup>; Yannik Zieger<sup>1</sup>; Martin Schwentenwein<sup>1</sup>; Shawn Allan<sup>2</sup>; <sup>1</sup>Lithoz GmbH; <sup>2</sup>Lithoz America LLC

**2:40 PM**

**Additive Manufacturing of ZrB<sub>2</sub>-ZrSi<sub>2</sub> Composites Using an Electron Beam Melting (EBM) Process:** Cheryl Xu<sup>1</sup>; <sup>1</sup>North Carolina State University

**3:00 PM**

**Process Development and Optimization for The Laser Powder Bed Fusion of WC-Ni Cermet Composites:** Edgar Mendoza Jimenez<sup>1</sup>; Baby Reeja-Jayan<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Equipment, Instrumentation and In-Situ Process Monitoring — Process Monitoring and Modeling Methods

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Joy Gockel, Colorado School of Mines; Sneha Prabha Narra, Carnegie Mellon University

**Tuesday PM | October 19, 2021**

**A121 | Greater Columbus Convention Center**

**Session Chair:** Sneha Prabha Narra, Carnegie Mellon University

**2:00 PM Invited**

**Combined In-situ Monitoring of Meltpool, Powder Layer, and Part Topography for Laser Powder Bed Fusion (LPBF) Based Metal Additive Manufacturing:** Xiayun Zhao<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**2:40 PM**

**Melt Pool Level Flaw Detection in Laser Hot Wire Additive Manufacturing Using a Trained Convolutional Long Short Term Memory Autoencoder:** Brandon Abranovic<sup>1</sup>; Sulagna Sarkar<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**3:00 PM**

**Materials Characterization of Anomalies Identified Through In-situ Process Monitoring Data Analytics:** Jonathan Ciero<sup>1</sup>; Dylan Christman<sup>1</sup>; Kyle Ryan<sup>2</sup>; Shuchi "SK" Khurana<sup>3</sup>; Thomas Spears<sup>2</sup>; Joy Gockel<sup>1</sup>; <sup>1</sup>Wright State University; <sup>2</sup>Open Additive, LLC; <sup>3</sup>Addiguru

**3:20 PM**

**Physics Guided Machine Learning DED Melt Pool Width Prediction:** Brett Diehl<sup>1</sup>; Clara Mock<sup>2</sup>; Lester Hitch<sup>2</sup>; Brandon McWilliams<sup>2</sup>; Berend Rinderspracher<sup>2</sup>; <sup>1</sup>Oak Ridge Associated Universities; <sup>2</sup>CCDC Army Research Laboratory

## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Ti-/Co-/Cr-/Cu-based Alloys

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

**Tuesday PM | October 19, 2021**

**A115 | Greater Columbus Convention Center**

**Session Chair:** Rangasayee Kannan, Oak Ridge National Laboratory

**2:00 PM**

**Designing a Beta Titanium Alloy with High Strength and Low Stiffness via Additive Manufacturing:** Yi Dan Wang<sup>1</sup>; Sravya Tekumalla<sup>1</sup>; Matteo Seita<sup>1</sup>; <sup>1</sup>Nanyang Technological University

**2:20 PM**

**Evaluation of In-situ Alloyed, Additively Manufactured GRCop-42:** David Scannapieco<sup>1</sup>; David Ellis<sup>2</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>NASA Glenn Research Center

# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: ICME Gaps: Material Property and Validation Data to Support Certification — Data Applications: Material Property and Validation Data to Support Certification

**Sponsored by:** TMS: Integrated Computational Materials Engineering Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Joshua Fody, NASA Langley Research Center; Edward Glaessgen, NASA Langley Research Center; Christopher Lang, NASA Langley Research Center; Greta Lindwall, KTH Royal Institute of Technology; Michael Sansoucie, NASA Marshall Space Flight Center; Mark Stoudt, National Institute of Standards and Technology

**Tuesday PM | October 19, 2021**  
**A114 | Greater Columbus Convention Center**

**Session Chairs:** Mark Stoudt, NIST; Seth Strayer, University of Pittsburgh

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**2:00 PM Invited**  
**Lessons Learned from Calibration and Validation of Process Models for Laser Powder Bed Fusion:** *Albert To<sup>1</sup>; Florian Dugast<sup>1</sup>; Seth Strayer<sup>1</sup>; Wen Dong<sup>1</sup>; Xuan Liang<sup>1</sup>; Qian Chen<sup>1</sup>; Hai Tran<sup>1</sup>; Shawn Hinnebusch<sup>1</sup>; Xavier Jimenez<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**2:30 PM**  
**Transferability of Terrestrial Development of Metal Additive to Extraterrestrial Applications:** *Judy Schneider<sup>1</sup>; <sup>1</sup>University of Alabama at Huntsville*

**2:50 PM Invited**  
**ICME Gap Analysis for Materials Design and Process Optimization in Additive Manufacturing:** *Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**3:20 PM Invited**  
**Enabling Quality Assurance by Completing the Process-Property-Performance Paradigm for Additive Manufacturing:** *Peter Collins<sup>1</sup>; <sup>1</sup>Iowa State University*

**3:50 PM**  
**An ICME Approach for Designing Appropriate Heat Treatments in Additively Manufactured Nitrogen Atomized 17-4PH Stainless Steel:** *James Zuback<sup>1</sup>; Mark Stoudt<sup>1</sup>; Daniel Gopman<sup>1</sup>; Maureen Williams<sup>1</sup>; Carelyn Campbell<sup>1</sup>; <sup>1</sup>NIST*

**4:10 PM Keynote**  
**Critical Issues and Gaps in Testing and Characterization Data for Computational Materials in Qualification and Certification of Additively Manufactured Metallic Materials:** *Michael Gorelik<sup>1</sup>; Edward Glaessgen<sup>2</sup>; <sup>1</sup>Federal Aviation Administration; <sup>2</sup>NASA Langley Research Center*

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — Session III

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**Tuesday PM | October 19, 2021**  
**A120 | Greater Columbus Convention Center**

**Session Chair:** Ulf Ackelid, Freemelt AB

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**2:00 PM**  
**Examining the Role of Parent Grain Orientations on the Texture and Physical Properties of Additively Manufactured Ti 6-4 Alloys:** *Michael Hjelmstad<sup>1</sup>; Pat Trimby<sup>1</sup>; <sup>1</sup>Oxford Instruments*

**2:20 PM**  
**On the Use of Defects as Microstructural Informants in EBM Ti-6Al-4V:** *Katie O'Donnell<sup>1</sup>; Maria Quintana<sup>1</sup>; Matthew Kenney<sup>1</sup>; Peter Collins<sup>1</sup>; <sup>1</sup>Iowa State University*

**2:40 PM**  
**Use of Small Geometry Specimens to Determine the Fracture and Fatigue Crack Growth Properties of Additively Manufactured Ti-6Al-4V via DED Technique for Repair:** *Sammy Ojo<sup>1</sup>; Sulochana Shrestha<sup>1</sup>; Joseph El Rassi<sup>1</sup>; Manigandan Kannan<sup>1</sup>; Gregory Morscher<sup>1</sup>; Andrew Gyekenyesi<sup>1</sup>; Onome Scott-Emuakpor<sup>1</sup>; <sup>1</sup>University of Akron*

**3:00 PM**  
**Vibration Bending Fatigue Analysis of Additively Repaired Ti-6Al-4V Airfoil Blades:** *Lucas Smith<sup>1</sup>; Onome Scott-Emuakpor<sup>2</sup>; Joy Gockel<sup>3</sup>; Dino Celli<sup>2</sup>; Brian Runyon<sup>2</sup>; <sup>1</sup>Ohio Aerospace Institute; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>Wright State University*

**3:20 PM**  
**Influence of Foreign-Object Damage on the High Cycle Fatigue Properties of Direct Energy Deposition Repaired Ti-6Al-4V:** *Sulochana Shrestha<sup>1</sup>; Manigandan Kannan<sup>1</sup>; Gregory Morscher<sup>1</sup>; Andrew Gyekenyesi<sup>2</sup>; Onome Scott-Emuakpor<sup>3</sup>; <sup>1</sup>University of Akron; <sup>2</sup>Ohio Aerospace Institute; <sup>3</sup>Aerospace Systems Directorate*

## ENERGY

### Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments — Thermomechanical Testing and In Situ Environments

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Tuesday PM | October 19, 2021**  
**A215 | Greater Columbus Convention Center**

**Session Chairs:** Charles Hirst, Massachusetts Institute of Technology; Michael Short, Massachusetts Institute of Technology

#### 2:00 PM Invited

**Development of In-situ Atomic Scale Defect Spectroscopy during Ion Irradiation:** *Farida Selim*<sup>1</sup>; A Jones<sup>1</sup>; Y Wang<sup>2</sup>; S Agarwal<sup>1</sup>; H Kim<sup>2</sup>; P Hosemann<sup>3</sup>; B Uberuaga<sup>2</sup>; <sup>1</sup>Bowling Green State University; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>University of California Berkeley

#### 2:20 PM

**In-situ Radiological Containment Sample Environments: A review of Capability and Compromises at X-ray and Neutron Sources:** *D. Travis Carver*<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

#### 2:40 PM

**Finding a Balance in FeCrAl Alloys: Utilizing Advanced Characterization, Testing, and Machine Learning to Balance Properties:** *Andrew Hoffman*<sup>1</sup>; Vipul Gupta<sup>1</sup>; Daniel Ruscitto<sup>1</sup>; Bojun Feng<sup>1</sup>; Sayan Ghosh<sup>1</sup>; Raul Rebak<sup>1</sup>; <sup>1</sup>GE Research

#### 3:00 PM Invited

**Revealing Hidden Defects via Stored Energy Measurements of Radiation Damage:** *Charles Hirst*<sup>1</sup>; Fredric Granberg<sup>2</sup>; Penghui Cao<sup>3</sup>; Scott Middlemas<sup>4</sup>; R. Scott Kemp<sup>1</sup>; Ju Li<sup>1</sup>; Kai Nordlund<sup>2</sup>; Michael Short<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology; <sup>2</sup>University of Helsinki; <sup>3</sup>University of California, Irvine; <sup>4</sup>Idaho National Laboratory

#### 3:20 PM Invited

**Moduli Measurements of Fuels and Cladding Materials via Resonant Ultrasound Spectroscopy:** *Tarik Saleh*<sup>1</sup>; Mathew Hayne<sup>1</sup>; Scarlett Widgeon Paisner<sup>1</sup>; Joshua White<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

#### 3:40 PM

**In Situ Transient Grating Spectroscopy for Rapid Radiation Tolerance Characterization:** *Benjamin Dacus*<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Session II

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**Tuesday PM | October 19, 2021**  
**A223 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

#### 2:00 PM Keynote

**RF Radomes and IR Windows for Hypersonic Flight: Material Requirements and Development of Ceramic Processing Routes for Success:** *Rodney Trice*<sup>1</sup>; Averyonna Kimery<sup>1</sup>; Ashwin Sivakumar<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; Carlos Martinez<sup>2</sup>; Andrew Schlup<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>UES

#### 2:30 PM

**Novel Non-aqueous Gelcasting of UHTCs for Advanced Complex Shape Manufacturing:** *Julia Goyer*<sup>1</sup>; Carolina Tallon<sup>1</sup>; <sup>1</sup>Virginia Tech

#### 2:50 PM

**High Temperature Mixed Deposit and Oxidation Degradation of a Coated and Uncoated Ni-based Superalloys:** *Matthew Kovalchuk*<sup>1</sup>; Brian Gleeson<sup>1</sup>; <sup>1</sup>University of Pittsburgh

#### 3:10 PM

**Features of the Formation of the Structure and Properties of Corrosion-resistant Steel during Heat Treatment:** *Valeriy Mishchenko*<sup>1</sup>; Olha Bolsun<sup>1</sup>; Svitlana Mudra<sup>1</sup>; Sergiy Sheyko<sup>1</sup>; <sup>1</sup>Zaporizhzhia National University

## ELECTRONIC AND MAGNETIC MATERIALS

### Advances in Dielectric Materials and Electronic Devices — Modeling

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Ubic, Boise State University; Matjaž Spreitzer, Jožef Stefan Institute

**Tuesday PM | October 19, 2021**  
**B235 | Greater Columbus Convention Center**

**Session Chair:** Ruyan Guo, University of Texas at San Antonio

#### 2:00 PM

**Investigation of Electroplated 3D Printed Antennas:** *Muneer Barnawi*<sup>1</sup>; Trenton Cersoli<sup>1</sup>; Kerry Johnson<sup>1</sup>; Edward Burden<sup>1</sup>; Eric MacDonald<sup>1</sup>; Pedro Cortes<sup>1</sup>; <sup>1</sup>Youngstown State University

#### 2:20 PM

**NSMM Modeling of Materials, Including Dipole Engineered Novel Relaxors:** *Steven Tidrow*<sup>1</sup>; <sup>1</sup>Alfred University



# Technical Program

2:40 PM

**Topological Insulator Design for Quantum Computers Targeting BSTS Single Crystal Fabrication:** *Husain Alnaser*<sup>1</sup>

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## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Ferrous Metallurgy — Developments in Testing and Processing

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Emmanuel De Moor, Colorado School of Mines; Kishlay Mishra, Nucor Castrip Arkansas LLC; Lijia Zhao, ArcelorMittal Global R&D

**Tuesday PM | October 19, 2021**  
**A210 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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2:00 PM

**Effect of Alloying Content on Fractional Softening Behavior and Microstructural Evolution During Double-twist Torsion Testing of Microalloyed Steels:** *Trevor Ballard*<sup>2</sup>; Emmanuel De Moor<sup>1</sup>; <sup>1</sup>Advanced Steel Processing and Products Research Center, Colorado School of Mines

2:20 PM

**The Effect of Energy-power Parameters of Hot Rolling on Structure and Properties of Low Alloyed Steels:** *Valeriy Mishchenko*<sup>1</sup>; Sergiy Sheyko<sup>1</sup>; Vadim Shalomeev<sup>1</sup>; <sup>1</sup>Zaporizhzhia National University

2:40 PM

**Reducing the Effects of Texture on Phase Fraction Measurement of Retained Austenite Using X-ray Diffraction:** *Michael Cox*<sup>1</sup>; Adam Creuziger<sup>2</sup>; Kip Findley<sup>1</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>National Institute of Standards and Technology

3:00 PM

**3D Non-destructive Characterization of Texture Evolution in Electrical Steels with Lab-based Diffraction Contrast Tomography:** Jun Sun<sup>1</sup>; Florian Bachmann<sup>1</sup>; Jette Oddershede<sup>1</sup>; Hrishikesh Bale<sup>2</sup>; William Harris<sup>3</sup>; Erik Lauridsen<sup>1</sup>; <sup>1</sup>Xnovo Technology; <sup>2</sup>Carl Zeiss X-ray Microscopy; <sup>3</sup>Carl Zeiss Microscopy, LLC

3:20 PM

**Hole Expansion Performance of Three High Strength Steels: Observation of Room Temperature Strain Ageing Phenomena:** Rachael Stewart<sup>1</sup>; Mike Settle<sup>1</sup>; <sup>1</sup>Cleveland-Cliffs Steel Corporation

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## NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — Nanocomposites & 2D Materials

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**Tuesday PM | October 19, 2021**  
**B240/241 | Greater Columbus Convention Center**

**Session Chairs:** Sanjay Mathur, University of Cologne; Haitao Zhang, University of North Carolina at Charlotte

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2:00 PM Invited

**2d Crystalline Donors and Acceptors: Modulation Doping in Atomically-thin Heterostructures:** *Erik Henriksen*<sup>1</sup>; <sup>1</sup>Washington University in St. Louis

2:30 PM

**Thickness-dependent Piezoelectric Property of Two-dimensional Zinc Oxide Nanosheets with Unit Cell Resolution:** *Corey Carlos*<sup>1</sup>; Yizhan Wang<sup>1</sup>; Jingyu Wang<sup>1</sup>; Jun Li<sup>1</sup>; Xudong Wang<sup>1</sup>; <sup>1</sup>University of Wisconsin - Madison

2:50 PM

**Processing and Mechanical Properties of 3YSZ-AL<sub>2</sub>O<sub>3</sub> Core-Shell Nanocomposite Ceramics:** *Kevin Anderson*<sup>1</sup>; Benjamin Greenberg<sup>1</sup>; James Wollmershauser<sup>1</sup>; Boris Feigelson<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory

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## PROCESSING AND MANUFACTURING

### Development of Light Weight Alloys and Composites — Microstructure and Properties: Composites III

**Program Organizers:** Ramasis Goswami, Naval Research Laboratory; Nikhil Gupta, New York University; Tanjore Jayaraman, University of Michigan-Dearborn; Aashish Rohatgi, Pacific Northwest National Laboratory

**Tuesday PM | October 19, 2021**  
**A214 | Greater Columbus Convention Center**

**Session Chairs:** Tanjore Jayaraman, College of Engineering and Computer Science, University of Michigan-Dearborn; Ramasis Goswami, NRL

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2:00 PM

**Development of Bulk Nanocrystalline Aluminum Materials with Enhanced Mechanical Properties:** Pradeep Menezes<sup>1</sup>; Sridhar Lanka<sup>1</sup>; Raven Maccione<sup>1</sup>; Bhaskar Vadlamani<sup>1</sup>; Manoranjan Misra<sup>1</sup>; <sup>1</sup>University of Nevada Reno

**2:30 PM**

**Tensile Properties of Epoxy Composites Reinforced with Continuous Mixed Natural Fibers:** *Frederico Margem*<sup>1</sup>; Niander Aguiar<sup>1</sup>; Fernanda Rangel<sup>1</sup>; João Dornelas<sup>1</sup>; <sup>1</sup>Uniredentor

**3:00 PM**

**The Effect of Multiple Age Treatment on Mechanical Properties of 7075 Al Alloy:** *AHM Esfakur Rahman*<sup>1</sup>; Issam Abu-Mahfouz<sup>1</sup>; Amit Banerjee<sup>1</sup>; <sup>1</sup>Pennsylvania State University Harrisburg

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## IRON AND STEEL (FERROUS ALLOYS)

### Developments in Plate and Line Pipe Steels — Developments in Plate and Line Pipe Steels

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Ashish Singh, Nucor Steel Arkansas; Pello Uranga, CEIT and TECNUN (University of Navarra)

**Tuesday PM | October 19, 2021**

**A211 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**2:00 PM**

**Modified Charpy V-notch Testing of Wind Tower Steels:** *Keith Taylor*<sup>1</sup>; Laura Dawson<sup>2</sup>; Matthew Werner<sup>1</sup>; <sup>1</sup>SSAB Americas; <sup>2</sup>Virginia Polytechnic Institute and State University

**2:20 PM**

**The Formation of Structure and Properties of Low-alloyed Steels in Hot Deformation Process:** *Valeriy Mishchenko*<sup>1</sup>; Sergiy Sheyko<sup>1</sup>; Vadim Shalomoev<sup>2</sup>; <sup>1</sup>Zaporizhzhia National University; <sup>2</sup>National University "Zaporizhzhia Polytechnic"

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## ENERGY

### Energy Materials for Sustainable Development — Storage Batteries I

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

**Tuesday PM | October 19, 2021**

**A216 | Greater Columbus Convention Center**

**Session Chairs:** Jeffrey Fergus, Auburn University; Giovanni Fanchini, University of Western Ontario

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**2:00 PM Invited**

**Challenges and Opportunities of Oxide-based Cathodes for Aqueous Zn-ion Batteries:** *Kevin Huang*<sup>1</sup>; <sup>1</sup>University of South Carolina

**2:30 PM**

**Reducing the Sintering Temperature of Ceramic Solid-State Batteries with the Cold Sintering Process:** *Zane Grady*<sup>1</sup>; Joo-Hwan Seo<sup>1</sup>; Arnaud Ndayishimiye<sup>1</sup>; Clive Randall<sup>1</sup>; <sup>1</sup>The Pennsylvania State University

**2:50 PM Invited**

**Nanoscale Geometry and Point Defects in Supercapacitor Electrodes:** *Scott Mixture*<sup>1</sup>; <sup>1</sup>Alfred University

**3:10 PM**

**Doping Study of Nanoscale Lithium Cobalt Oxide Surfaces and Grain Boundaries:** *Spencer Dahl*<sup>1</sup>; Blas Uberuaga<sup>2</sup>; Ricardo Castro<sup>1</sup>; <sup>1</sup>University of California, Davis; <sup>2</sup>Los Alamos National Laboratory

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## CERAMIC AND GLASS MATERIALS

### Engineering Ceramics: Microstructure-Property- Performance Relations and Applications — Engineering Ceramics

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Young-Wook Kim, University of Seoul; Hua-Tay Lin, Guangdong University of Technology; Junichi Tatami, Yokohama National University

**Tuesday PM | October 19, 2021**

**B233 | Greater Columbus Convention Center**

**Session Chair:** Ivar Reimanis, Colorado School of Mines

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**2:00 PM Invited**

**Tracking the State of Transition Elements Ni and Fe in Oxide Microstructures:** *Michael Knight*<sup>1</sup>; *Ivar Reimanis*<sup>1</sup>; Dylan Jennings<sup>1</sup>; Sandrine Ricote<sup>1</sup>; Wolfgang Rheinheimer<sup>2</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Julich Research Center

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## CERAMIC AND GLASS MATERIALS

### Glasses and Optical Materials: Current Issues and Functional Applications — ACerS Alfred R. Cooper Award Session

**Sponsored by:** ACerS Basic Science Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Delia Brauer, Otto Schott Institute of Materials Research

**Tuesday PM | October 19, 2021**

**B231 | Greater Columbus Convention Center**

**Session Chair:** Steve Martin, Iowa State University

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**2:00 PM Introductory Comments**

**2:10 PM Invited**

**Cooper Distinguished Lecture: Structure and Ion Dynamics in Glass:** *Efstathios Kamitsos*<sup>1</sup>; <sup>1</sup>Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation

# Technical Program

2:50 PM Question and Answer Period/Presentation of Award

3:00 PM Invited

**Cooper Scholar: Study of the Anomalous Viscosity in Invert NaPSO Glass for the Development of Thin Solid-state Electrolytes:** *Jacob Lovi*<sup>1</sup>; <sup>1</sup>Iowa State University

3:20 PM Question and Answer Period/Presentation of Award

3:30 PM Invited

**Cooper Scholar 1st Runner-up: Relationship between Number of Non-bridging Oxygens and Ionic Conductivity Discontinuity in xLi<sub>2</sub>O-(1-x) B<sub>2</sub>O<sub>3</sub>, with x = 0.67:** *Graham Beckler*<sup>1</sup>; <sup>1</sup>Coe College

3:50 PM Question and Answer Period/Presentation of Award

4:00 PM Invited

**Cooper Scholar 2nd Runner-up: Solution-processed Telluride Glass for Far-infrared Applications:** *Lauren Moghimi*<sup>1</sup>; <sup>1</sup>University of Arizona

4:20 PM Question and Answer Period/Presentation of Award

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## FUNDAMENTALS AND CHARACTERIZATION

### Grain Boundaries, Interfaces, and Surfaces in Ceramics: Fundamental Structure—Property—Performance Relationships — Field Assisted Processes and Mechanics

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Rheinheimer Wolfgang, Forschungszentrum Jülich; Catherine Bishop, University of Canterbury; Shen Dillon, University of California, Irvine; Ming Tang, Rice University; John Blendell, Purdue University; Wayne Kaplan, Technion - Israel Institute of Technology; Melissa Santala, Oregon State University

**Tuesday PM | October 19, 2021**  
**B244/245 | Greater Columbus Convention Center**

**Session Chairs:** Xufei Fang, TU Darmstadt; Timofey Frolov, Lawrence Livermore National Laboratory

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2:00 PM

**Hall-etch Behavior in Stoichiometric and Al-rich Nanocrystalline ZnAl<sub>2</sub>O<sub>4</sub>:** *Luis Sotelo Martin*<sup>1</sup>; Ricardo Castro<sup>1</sup>; <sup>1</sup>University of California, Davis

2:20 PM

**Surface and Fracture Energy in Layered Ceramics:** *Oriol Gavalda-Diaz*<sup>2</sup>; Katharina Marquardt<sup>1</sup>; Eduardo Saiz<sup>2</sup>; Finn Giuliani<sup>1</sup>; <sup>1</sup>Imperial College London

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## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Processing and Properties I

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Tuesday PM | October 19, 2021**  
**B131 | Greater Columbus Convention Center**

**Session Chairs:** Oleg Senkov, Air Force Research Laboratory; Michael Mills, Ohio State University

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2:00 PM Invited

**Insights into the Deformation Processes of a Refractory Complex Concentrated Alloy Exhibiting B2-type Order:** Jean-Philippe Couzinie<sup>1</sup>; Milan Heczko<sup>2</sup>; Veronika Mazanova<sup>2</sup>; Oleg Senkov<sup>3</sup>; Rajarshi Banerjee<sup>4</sup>; Maryam Ghazisaeidi<sup>5</sup>; *Michael Mills*<sup>2</sup>; <sup>1</sup>Université Paris Est & Center for Electron Microscopy and Analysis, The Ohio State University; <sup>2</sup>Center for Electron Microscopy and Analysis, The Ohio State University; <sup>3</sup>Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB; <sup>4</sup>University of North Texas; <sup>5</sup>The Ohio State University

2:20 PM Invited

**Deformation Behavior in the Refractory High-entropy Alloys:** *Chanho Lee*<sup>1</sup>; George Kim<sup>2</sup>; Yi Chou<sup>3</sup>; Michael Gao<sup>4</sup>; Ke An<sup>5</sup>; Gian Song<sup>6</sup>; Yi-Chia Chou<sup>3</sup>; Wei Chen<sup>2</sup>; Saryu Fensin<sup>1</sup>; Peter Liaw<sup>7</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Illinois Institute of Technology; <sup>3</sup>National Chiao Tung University; <sup>4</sup>National Energy Technology Laboratory/Leidos Research Support Team; <sup>5</sup>Oak Ridge National Laboratory; <sup>6</sup>Kongju National University; <sup>7</sup>University of Tennessee

2:40 PM

**A Low-temperature Chemical/Powder Metallurgical Route for Generating Fine-grained Refractory Complex Concentrated Alloys:** *Kenneth Sandhage*<sup>1</sup>; Sona Avetian<sup>1</sup>; Mario Caccia<sup>1</sup>; Michael Titus<sup>1</sup>; <sup>1</sup>Purdue University

3:00 PM

**The Cyclic Plastic Strain Localization and the Fatigue Crack Initiation in Equiatomic CrCoNi Medium-entropy Alloy:** *Veronika Mazanova*<sup>1</sup>; Milan Heczko<sup>1</sup>; Connor Slone<sup>2</sup>; Shih Mulaine<sup>3</sup>; Easo P. George<sup>3</sup>; Maryam Ghazisaeidi<sup>1</sup>; Jaroslav Polak<sup>4</sup>; Michael J. Mills<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Exponent; <sup>3</sup>Oak Ridge National Laboratory; <sup>4</sup>Institute of Physics of Materials CAS

3:20 PM

**The Cyclic Plastic Response and the Fatigue Induced Microstructural Changes of Equiatomic CrCoNi Medium-entropy Alloy:** *Milan Heczko*<sup>1</sup>; Veronika Mazanova<sup>1</sup>; Connor Slone<sup>2</sup>; Ivo Kubena<sup>3</sup>; Mulaine Shih<sup>1</sup>; Tomáš Kruml<sup>3</sup>; Easo George<sup>4</sup>; Maryam Ghazisaeidi<sup>1</sup>; Jaroslav Polák<sup>3</sup>; Michael Mills<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Exponent; <sup>3</sup>Institute of Physics of Materials CAS; <sup>4</sup>Oak Ridge National Laboratory



### 3:40 PM Invited

**Discontinuous Precipitation Leading to Nano-rod Intermetallic Precipitates in High Entropy Alloys Results in an Excellent Strength-ductility Combination:** *Sriswaroop Dasari*<sup>1</sup>; Abhishek Sharma<sup>1</sup>; Bharat Gwalani<sup>1</sup>; Yao-Jen Chang<sup>2</sup>; Abhinav Jagetia<sup>1</sup>; Vishal Soni<sup>1</sup>; Stephane Gorsse<sup>3</sup>; An-Chou Yeh<sup>2</sup>; Rajarshi Banerjee<sup>1</sup>; <sup>1</sup>University Of North Texas; <sup>2</sup>National Tsing Hua University; <sup>3</sup>University of Bordeaux

### 4:00 PM

**Deformation Mechanisms in the Medium Entropy Alloy CoCrNi: Effects of Lattice Distortion and Chemical Short-range Order:** *Wurong Jian*<sup>1</sup>; Shuozi Xu<sup>1</sup>; Yanqing Su<sup>2</sup>; Irene Beyerlein<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>Utah State University

## SPECIAL TOPICS

### Input to the National Strategic Plan for Advanced Manufacturing – Discussion

**Program Organizers:** Said Jahanmir, Subcommittee on Advanced Manufacturing  
 National Science and Technology Council; James Warren, National Institute of Standards and Technology

**Tuesday PM | October 19, 2021**

**B130 | Greater Columbus Convention Center**

**3:00 PM Round Table Discussion:** Under the America COMPETES Act the federal government develops a national strategic plan for advanced manufacturing with stakeholder input from industry, academia non-profit organizations. The first of these quadrennial strategic plans was issued in 2018. Federal officials are seeking your input in the development of the 2022-2026 National Strategic Plan for Advanced Manufacturing. This Roundtable event is to solicit information from the Conference participants on where advanced manufacturing should go in the future and will follow questions to be issued in a public Request for Information from the White House Office of Science and Technology Policy.

## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III – Session III

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**Tuesday PM | October 19, 2021**

**B246 | Greater Columbus Convention Center**

**Session Chairs:** Bjorn Clausen, Los Alamos National Laboratory; Ben Morrow, Los Alamos National Laboratory

### 2:00 PM Invited

**In-situ Scattering Experiments Facilitating Development and Validation of Constitutive and Process Models:** *Bjorn Clausen*<sup>1</sup>; Donald Brown<sup>1</sup>; D. Travis Carver<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

### 2:40 PM

**Effect of Twin-twin Junctions on Slip-twin Interactions and Twin-twin Intersections:** *Jiaxiang Wang*<sup>1</sup>; M.Arul Kumar<sup>2</sup>; Krishna Yaddanapudi<sup>3</sup>; Subhash Mahajan<sup>3</sup>; Irene Beyerlein<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>University of California, Davis

### 3:00 PM

**The Interactions between Basal-precipitates and Propagating Twin Tips in AZ91:** *Brandon Leu*<sup>1</sup>; Mariyappan Kumar<sup>2</sup>; Irene Beyerlein<sup>2</sup>; <sup>1</sup>University of California-Santa Barbara; <sup>2</sup>Los Alamos National Lab

### 3:20 PM

**Fluctuations in the Generalized Planar Fault Energy Landscape in Concentrated FCC Solid Solutions:** *Matthew Daly*<sup>1</sup>; Ritesh Jagatramka<sup>1</sup>; Chu Wang<sup>1</sup>; <sup>1</sup>University of Illinois-Chicago

### 3:40 PM

**First-principles Study of the Effect of Al and Hf Impurities on Co<sub>3</sub>W Antiphase Boundary Energies:** *Chiraag Nataraj*<sup>1</sup>; Ruoshi Sun<sup>2</sup>; Christopher Woodward<sup>3</sup>; Axel van de Walle<sup>1</sup>; <sup>1</sup>Brown University; <sup>2</sup>University of Virginia; <sup>3</sup>Air Force Research Lab

### 4:00 PM

**Thermodynamic Modeling of the Ga-Ni System Using the Third Generation Gibbs Free Energy Function for Pure Elements:** *Liangyan Hao*<sup>1</sup>; Chen Shen<sup>2</sup>; Hongbin Zhang<sup>2</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Technische Universität of Darmstadt

### 4:20 PM Invited

**Co-development of Experiment and Simulation to Observe Dynamic Behavior in Metals in Complex Loading Environments:** *Benjamin Morrow*<sup>1</sup>; Virginia Euser<sup>1</sup>; Clarissa Yablinsky<sup>1</sup>; Nicholas Denissen<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

## CERAMIC AND GLASS MATERIALS

### Manufacturing and Processing of Advanced Ceramic Materials – Processing of Oxide Ceramics

**Sponsored by:** ACerS Manufacturing Division

**Program Organizers:** Bai Cui, University of Nebraska-Lincoln; James Hemrick, Oak Ridge National Laboratory; Mike Alexander, Allied Mineral Products; Eric Faierson, Quad City Manufacturing Laboratory/Western Illinois University; Keith DeCarlo, Blasch Precision Ceramics

**Tuesday PM | October 19, 2021**

**B234 | Greater Columbus Convention Center**

**Session Chair:** Yiquan Wu, Alfred University

### 2:00 PM Invited

**Effects of Sintering Additive and Oxygen Partial Pressure on Solid-state Single-crystal Growth of YAG Ceramics:** *Iva Milisavljevic*<sup>1</sup>; Guangran Zhang<sup>1</sup>; Yiquan Wu<sup>1</sup>; <sup>1</sup>Alfred University

### 2:40 PM

**Unique Technological Advantages and Progress towards Manufacturing Scale-up:** *Sun Hwi Bang*<sup>1</sup>; Clive Randall<sup>1</sup>; <sup>1</sup>Pennsylvania State University



# Technical Program

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## BIOMATERIALS

### Next Generation Biomaterials — Session II

**Sponsored by:** ACerS Bioceramics Division, TMS Biomaterials Committee

**Program Organizers:** Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

**Tuesday PM | October 19, 2021**  
**A224 | Greater Columbus Convention Center**

**Session Chairs:** Anna Bull, University of Tennessee Space Institute; Begoña Ferrari, Instituto de Cerámica y Vidrio del CSIC

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**2:00 PM Invited**  
**A Breath Test for COVID-19:** *Pelagia Gouma*<sup>1</sup>; <sup>1</sup>The Ohio State University

**2:20 PM Invited**  
**Reducing Intraoperative Fogging of Laparoscopes with Diamond-like Carbon Thin Films:** *Anna Bull*<sup>1</sup>; Christopher Haycock<sup>2</sup>; Chad Bond<sup>3</sup>; Russell Leonard<sup>3</sup>; Todd Giorgio<sup>2</sup>; Jacqueline Johnson<sup>3</sup>; <sup>1</sup>University of Tennessee Space Institute; <sup>2</sup>Vanderbilt University; <sup>3</sup>UT Space Institute

**2:40 PM**  
**Investigation of Biodegradable Mg-Li Quaternary Alloys with Improved Uniform Degradation:** *Chiamaka Okafor*<sup>1</sup>; Norman Munroe<sup>1</sup>; <sup>1</sup>Florida International University

**3:00 PM**  
**Mechanical Behavior of Bonded-PDMS for Biological Payloads in Microgravity:** *Annaliza Perez-Torres*<sup>1</sup>; <sup>1</sup>Space Tango

**3:20 PM**  
**Comparative Evaluation of Nutrient Composition in Cow Hornwaste and Some Commercially Available Fish Feed as Supplement in Aquaculture:** *Ita Uwidia*<sup>1</sup>; Osalodion Uwidia<sup>1</sup>; <sup>1</sup>University of Benin

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## CERAMIC AND GLASS MATERIALS

### Phase Transformations in Ceramics: Science and Applications — Computation and Predictions

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Scott McCormack, University of California, Davis; Pankaj Sarin, Oklahoma State University; Sanjay V. Khare, University of Toledo; Waltraud Kriven, University of Illinois at Urbana-Champaign

**Tuesday PM | October 19, 2021**  
**B230 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**2:00 PM**  
**Effects of S Doping on the Mechanical and Opto-electronic Properties of Cu<sub>2</sub>CdGeSe<sub>4</sub>:** Victor Barone<sup>1</sup>; Bishal Dumre<sup>1</sup>; Randall Ellingson<sup>1</sup>; Sanjay Khare<sup>1</sup>; <sup>1</sup>The University of Toledo

**2:20 PM**

**Nanostructured Spinel Ferrite Ceramics: Structure and Magnetic Properties:** *Suraj Mullurkara*<sup>1</sup>; Y. Wang<sup>1</sup>; A. Talaat<sup>1</sup>; W. Xiong<sup>1</sup>; J.K. Lee<sup>1</sup>; P.R. Ohodnicki<sup>1</sup>; <sup>1</sup>University of Pittsburgh

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## BIOMATERIALS

### Porous Materials for Biomedical Applications — Session I

**Sponsored by:** ACerS Bioceramics Division

**Program Organizers:** Usman Liaqat, National University of Sciences and Technology; Chuanbin Mao, University of Oklahoma; Mingying Yang, Zhejiang University

**Tuesday PM | October 19, 2021**  
**A222 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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**2:00 PM**  
**Multifunctional Artificial Artery from Direct 3D Printing with Built-in Ferroelectricity and Tissue-matching Modulus for Real-time Sensing and Occlusion Monitoring:** *Jun Li*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**2:20 PM**  
**Synthesis and Characterization of Porous Diopside Scaffold Synthesized Using Rice Husk as a Space Holder Material for Orthopedic Application:** *Mayank Yadav*<sup>1</sup>; Vaibhav Pandey<sup>1</sup>; Jyoti Kumari<sup>1</sup>; Kalyani Mohanta<sup>1</sup>; Vinay Singh<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (BHU), Varanasi

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## PROCESSING AND MANUFACTURING

### Powder Metallurgical Components in High Performance Applications — Session I

**Sponsored by:** TMS Powder Materials Committee

**Program Organizers:** Peng Cao, The University of Auckland; Hanadi Salem, American University in Cairo; Paul Prichard, Kennametal Inc.; Matthew Osborne, Global Advanced Metals; James Paramore, US Army Research Laboratory

**Tuesday PM | October 19, 2021**  
**A213 | Greater Columbus Convention Center**

**Session Chair:** James Paramore, United States Army Research Laboratory

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**2:00 PM**  
**Development of Resistance Based Sintering for Metal Powders:** *Jerry Gould*<sup>1</sup>; James Cruz<sup>1</sup>; <sup>1</sup>Edison Welding Inst

**2:20 PM**  
**Dispersing Tailored Nanoparticles through Powder Metallurgy Consolidation:** *Bahrum Rocky*<sup>1</sup>; Rofiques Salehin<sup>2</sup>; Christopher Weinberger<sup>2</sup>; Steve Daniewicz<sup>1</sup>; Gregory Thompson<sup>1</sup>; <sup>1</sup>University of Alabama; <sup>2</sup>Colorado State University

## FUNDAMENTALS AND CHARACTERIZATION

### Probing Defect Properties and Behavior under Mechanical Deformation and Extreme Conditions — Defect-mediated Mechanical Performance and Damage Tolerance

**Sponsored by:** TMS Nanomechanical Materials Behavior Committee, TMS Nuclear Materials Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Zhe Fan, Lamar University; Tianyi Chen, Oregon State University; Shijun Zhao, City University of Hong Kong; Mitra Taheri, Johns Hopkins University; Yury Osetskiy, Oak Ridge National Laboratory

**Tuesday PM | October 19, 2021**  
**B140/141 | Greater Columbus Convention Center**

**Session Chairs:** Jian Wang, University of Nebraska-Lincoln; Tianyi Chen, Oregon State University

**2:00 PM Invited**

**Designing Metal and Amorphous Ceramic Composites for Extreme Conditions:** *Jian Wang*<sup>1</sup>; Binqiang Wei<sup>1</sup>; <sup>1</sup>University of Nebraska-Lincoln

**2:30 PM**

**Estimating the Strengthening Parameters for Irradiated Alloys Using Atomic Scale Dislocation Dynamics:** *Osetskiy Yury*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**2:50 PM**

**Investigating Deformation Mechanisms in Ni-based Superalloys with Compact 'L' Coprecipitates:** *Semanti Mukhopadhyay*<sup>1</sup>; Hariharan Sriram<sup>1</sup>; Richard DiDomizio<sup>2</sup>; Andrew Detor<sup>2</sup>; Robert Hayes<sup>3</sup>; Gopal B. Viswanathan<sup>1</sup>; Yunzhi Wang<sup>1</sup>; Michael Mills<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>GE Global Research Center; <sup>3</sup>Metals Technology Inc.

**3:10 PM**

**Nanomechanical Properties of Neutron Irradiated Austenitic Steels:** *Tianyi Chen*<sup>1</sup>; Mack Cullison<sup>1</sup>; <sup>1</sup>Oregon State University

**3:30 PM Break**

**3:50 PM**

**Local Phase Transformation Strengthening in Ni-based Superalloys:** *Ashton Egan*<sup>1</sup>; Fei Xue<sup>2</sup>; Timothy Smith<sup>3</sup>; Longsheng Feng<sup>1</sup>; Shakthipriya Baskar<sup>1</sup>; Emmanuelle Marquis<sup>2</sup>; Yunzhi Wang<sup>1</sup>; Maryam Ghazisaeidi<sup>1</sup>; Michael Mills<sup>1</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>University of Michigan; <sup>3</sup>NASA Glenn Research Center

**4:10 PM**

**Phase-field Modeling of Electromigration-mediated Void Migration and Coalescence under Mechanical and Current-stressing in Interconnect Lines:** *William Farmer*<sup>1</sup>; Sree Vemulapalli<sup>1</sup>; Kumar Ankit<sup>1</sup>; <sup>1</sup>Arizona State University

**4:30 PM**

**Mechanical and Microstructural Responses of Severe-plastic Deformed High Entropy Alloys under Irradiation:** *Spencer Doran*<sup>1</sup>; Tracey Spoerer<sup>1</sup>; Megumi Kawasaki<sup>1</sup>; Youxing Chen<sup>2</sup>; Di Chen<sup>3</sup>; Tianyi Chen<sup>1</sup>; <sup>1</sup>Oregon State University; <sup>2</sup>University of North Carolina Charlotte; <sup>3</sup>University of Houston

## SPECIAL TOPICS

### ACerS Robert B. Sosman Award Symposium: Bridging the Gap between Atomistic and Continuum Approaches to Interface Science — Sosman I

**Sponsored by:** ACerS Basic Science Division

**Program Organizer:** John Blendell, Purdue University

**Wednesday AM | October 20, 2021**  
**B130 | Greater Columbus Convention Center**

**Session Chair:** John Blendell, Purdue University

**8:00 AM Introductory Comments**

**8:10 AM Invited**

**Stressing Surfaces and Interfaces to Change Microstructure:** *Klaus van Benthem*<sup>1</sup>; <sup>1</sup>University of California, Davis

**8:40 AM Invited**

**Atomic Structure of Two Phases of a Cu Tilt Grain Boundary Resolved by Scanning Transmission Electron Microscopy:** *Gerhard Dehm*<sup>1</sup>; Thorsten Meiners<sup>1</sup>; Jazmin Duarte<sup>1</sup>; Timofey Frolov<sup>2</sup>; Christian Liebscher<sup>1</sup>; <sup>1</sup>MPI Eisenforschung; <sup>2</sup>Lawrence Livermore National Laboratory

**9:10 AM Invited**

**Formation/Migration of Faceted Boundaries and Grain Growth Behavior in Ni:** *Suk-Joong Kang*<sup>1</sup>; <sup>1</sup>KAIST

**9:40 AM Invited**

**Charged Interfaces: Equilibrium, Phase Transitions, and Microstructural Evolution:** *KSN Vikrant*<sup>1</sup>; *Edwin Garcia*<sup>1</sup>; <sup>1</sup>Purdue University

**10:10 AM Break**

**10:30 AM Invited**

**Microstructure Evolution in Thin Film Yttria-doped Barium Zirconate:** *Dylan Jennings*<sup>1</sup>; *Ivar Reimanis*<sup>1</sup>; Sandrine Ricote<sup>1</sup>; Jose Santiso<sup>2</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Catalan Institute of Nanoscience and Nanotechnology, ICN2

**11:00 AM Invited**

**FCC Films on c-sapphire: Why Do Single Elements and High Entropy Alloys Adopt the Same Orientation Relationships?:** *Dominique Chatain*<sup>1</sup>; <sup>1</sup>CNRS

**11:30 AM Invited**

**Combining Atomistic to Thermodynamic Modeling with Machine Learning and Advanced Microscopy to Understand General Grain Boundaries and Interfaces:** *Jian Luo*<sup>1</sup>; <sup>1</sup>University of California, San Diego

# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of High and Ultra-High Temperature Ceramics and Composites: Processing, Characterization and Testing — Polymer-derived Ceramics (PDCs) and Novel Processing Methods

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Corson Cramer, Oak Ridge National Laboratory; Greg Hilmas, Missouri University of Science and Technology; Lisa Rueschhoff, Air Force Research Laboratory

**Wednesday AM | October 20, 2021**  
**A111 | Greater Columbus Convention Center**

**Session Chair:** William Costakis, Air Force Research Labs

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**10:00 AM**

**Advanced Polymer-derived (Ultra)-high-temperature Resistant Ceramics and Ceramic Nanocomposites for Additive Manufacturing:** *Ralf Riedel*<sup>1</sup>; <sup>1</sup>TU Darmstadt

**10:30 AM**

**Innovative Route for the 3D Printing of Hybrid Silicon Carbide/Carbon Fiber Nanocomposites:** *Saja Al-ajrash*; <sup>1</sup>

**10:50 AM**

**High Temperature Properties of Polymer-derived Ceramic Matrix Composites Fabricated via Additive Manufacturing:** *Tobias Schaedler*<sup>1</sup>; Kayleigh Porter<sup>1</sup>; Phuong Bui<sup>1</sup>; Ekaterina Stonkevitch<sup>1</sup>; Mark O'Masta<sup>1</sup>; <sup>1</sup>HRL Laboratories LLC

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Equipment, Instrumentation and In-Situ Process Monitoring — Imaging and Sensing Methods

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Joy Gockel, Colorado School of Mines; Sneha Prabha Narra, Carnegie Mellon University

**Wednesday AM | October 20, 2021**  
**A121 | Greater Columbus Convention Center**

**Session Chair:** Ulf Ackelid, Freemelt AB

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**8:00 AM**

**High-speed Observations and Quantification of Spatter in Laser Powder Bed Fusion:** *Christian Gobert*<sup>1</sup>; Jack Beuth<sup>1</sup>; Evan Diewald<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**8:20 AM**

**Advancing Measurement Science of Laser Powder Bed Fusion (LPBF) Process Monitoring Applying Thermal Imaging:** *Guadalupe Quirarte*<sup>1</sup>; Syed Zia Uddin<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**8:40 AM Invited**

**Innovative and Practical Approaches to Laser Powder Bed Fusion Sensing and Process Enhancement:** *John Middendorf*<sup>1</sup>; <sup>1</sup>Open Additive

**9:20 AM**

**In-situ Sensing in Processing Parameter Development for Bismuth Telluride Bulk Part Fabrication Using Laser Powder Bed Fusion:** *Kelly Rickert*<sup>1</sup>; Joy Gockel<sup>1</sup>; Sabrina D'Alesandro<sup>1</sup>; Saniya LeBlanc<sup>2</sup>; Tanvi Banerjee<sup>1</sup>; Alexander Groeger<sup>1</sup>; Joe Walker<sup>3</sup>; John Middendorf<sup>3</sup>; <sup>1</sup>Wright State University; <sup>2</sup>George Washington University; <sup>3</sup>Open Additive

**9:40 AM**

**Laser Powder Bed Fusion of Tall Thin Walled Structures: Dimensional Inaccuracy Due to Local Buckling, and In Situ Infrared Imaging for Early Failure Detection:** *Syed Zia Uddin*<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Other Miscellaneous Materials/Alloys

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

**Wednesday AM | October 20, 2021**  
**A115 | Greater Columbus Convention Center**

**Session Chair:** Roman Maev, University of Windsor

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**8:00 AM**

**3D Printing of the Half-Heusler Alloy Nb<sub>1-x</sub>CoSb, A Case for Ternary Thermoelectric Materials:** *Muath Almalki*<sup>1</sup>; David Dunand<sup>1</sup>; G. Jeffrey Snyder<sup>1</sup>; <sup>1</sup>Northwestern University

**8:20 AM**

**Defect Free Pure Molybdenum Processed through Electron Beam Melting:** *Patxi Fernandez-Zelaia*<sup>1</sup>; Chris Ledford<sup>1</sup>; Elizabeth Ellis<sup>2</sup>; Quinn Campbell<sup>1</sup>; Andres Marquez Rossy<sup>1</sup>; Michael Kirka<sup>1</sup>; Donovan Leonard<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Y-12 National Security Complex

**8:40 AM**

**Fabrication of Pure Tungsten Using Electron Beam Powder Bed Fusion:** *Christopher Ledford*<sup>1</sup>; Michael Kirka<sup>1</sup>; Patxi Fernandez-Zelaia<sup>1</sup>; Julio Ortega Rojas<sup>1</sup>; Andres Marquez Rossy<sup>1</sup>; Yutai Kato<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**9:00 AM**

**Design of Wire-arc Additive Manufacturing of Functionally Graded Alloy from P91 Steel to Inconel 740H Superalloy Using High-throughput Method:** *Xin Wang*<sup>1</sup>; Soumya Sridar<sup>1</sup>; Michael Klecka<sup>2</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Raytheon Technologies Research Center

**9:20 AM**

**Effect of Heat Treatment on Stainless Steel 420 And Inconel 718 Multi-material Structures Fabricated Laser Directed Energy Deposition:** *Beytullah Aydogan*<sup>1</sup>; Himanshu Sahasrabudhe<sup>1</sup>; <sup>1</sup>Michigan State University

**9:40 AM**

**Process-property Relationships of Additively Manufactured Multi-material NiZnCu-ferrite Soft Magnetic Composites:** *Caleb Andrews*<sup>1</sup>; Li Ma<sup>2</sup>; Ryan Carter<sup>2</sup>; Ian McCue<sup>2</sup>; Joseph Sopczak<sup>2</sup>; Mitra Taheri<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>The Johns Hopkins University Applied Physics Laboratory

## ADDITIVE MANUFACTURING

### Additive Manufacturing: Large-Scale Metal Additive Manufacturing — Advanced Manufacturing Process

**Program Organizers:** Yousub Lee, Oak Ridge National Laboratory; Antonio Ramirez, Ohio State University; Yashwanth Bandari, Meltio Inc.; Duckbong Kim, Tennessee Technological University; Wei Zhang, Ohio State University

**Wednesday AM | October 20, 2021**  
**A114 | Greater Columbus Convention Center**

**Session Chair:** Duckbong Kim, Tennessee Technological University

**8:00 AM**

**Manufacturing Large Scale Metal Parts via AM – Current and Future Directions:** Andrzej Nycz<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**8:40 AM**

**An Investigation of the Properties of Stamping Tool Inserts Manufactured Using a Novel Wire Deposition Additive Manufacturing Process:** Joy Forsmark<sup>1</sup>; Alan Gillard<sup>1</sup>; Sal Barriga<sup>2</sup>; Adam LaDelpha<sup>2</sup>; Henry Merrow<sup>2</sup>; Brian McCabe<sup>2</sup>; <sup>1</sup>Ford Motor Company; <sup>2</sup>Digital Alloys

**9:00 AM**

**Development of 3D Metal Printing for Toolmaking:** Felix Gemse<sup>1</sup>; Danny Lubosch<sup>2</sup>; Olaf Penning<sup>3</sup>; Edgar Fries<sup>4</sup>; Enrico Danz<sup>5</sup>; <sup>1</sup>Günter-Köhler-Institute GmbH; <sup>2</sup>Gefertec GmbH; <sup>3</sup>Hermann Fliess & Co. GmbH; <sup>4</sup>Fraunhofer Institute for Production Systems and Design Technology IPK; <sup>5</sup>SWM Werkzeugfabrik GmbH & Co.KG

**9:20 AM**

**Hybrid Metal Manufacturing of Large Freeform Geometries:** Bradley Jared<sup>1</sup>; William Hamel<sup>1</sup>; Tony Schmitz<sup>1</sup>; Joshua Penney<sup>1</sup>; Leah Jacobs<sup>1</sup>; Aaron Cornelius<sup>1</sup>; Jake Dvorak<sup>1</sup>; Michael Buckley<sup>1</sup>; Greg Corson<sup>1</sup>; Eduardo Miramontes<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville

**9:40 AM**

**Novel Thermal Management Technique for Additive Manufacturing:** Robert Griffiths<sup>1</sup>; David Garcia<sup>2</sup>; Hang Yu<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute; <sup>2</sup>Pacific Northwest National Laboratory

**10:00 AM**

**High Deposition Rate Wire Arc Directed Energy Deposition of 316L for Pressure Retaining Components in Nuclear Applications:** Luc Hagen<sup>1</sup>; Stephen Tate<sup>2</sup>; Zhenzhen Yu<sup>1</sup>; Jonah Klemm-Toole<sup>1</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>EPRI

## ADDITIVE MANUFACTURING

### Additive Manufacturing: Mechanisms and Mitigation of Aqueous Corrosion and High-temperature Oxidation — Corrosion Assessment of Additively Manufactured Parts I

**Program Organizers:** Amir Mostafaei, Illinois Institute of Technology; Yashar Behnamian, University of Alberta; Bryan Webler, Carnegie Mellon University

**Wednesday AM | October 20, 2021**  
**A112 | Greater Columbus Convention Center**

**Session Chairs:** Amir Mostafaei, Illinois Institute of Technology; Bryan Webler, Carnegie Mellon University

**8:00 AM**

**SCC Behavior of IN 718 in BWR Conditions:** Amanda Leong<sup>1</sup>; Jinsuo Zhang<sup>1</sup>; George Pabis<sup>2</sup>; <sup>1</sup>Virginia Tech; <sup>2</sup>Nova Tech

**8:30 AM**

**Environmentally Assisted Cracking of AM718 Wire Arc Additively Deposited AM 718 – Role of Processing and Microstructure:** Ramgopal Thodla<sup>1</sup>; Badri Narayanan<sup>2</sup>; Hannah Sims<sup>2</sup>; Ben Schaeffer<sup>2</sup>; <sup>1</sup>DNV; <sup>2</sup>Lincoln Electric

**9:00 AM**

**Performance Evaluation of Oxidized Inconel 625 Made by Laser-assisted Additive Manufacturing:** Grace De Leon Nope<sup>1</sup>; Juan Alvarado-Orozco<sup>2</sup>; Guofeng Wang<sup>1</sup>; Brian Gleeson<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>CIDESI

**9:30 AM**

**Assessing the Printability and Oxidation Resistance of AM Built Al<sub>2</sub>CoCrFeNi with Directed Energy Deposition:** Jose Lol<sup>1</sup>; Bryan Webler<sup>1</sup>; Maarten De Boer<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — Session IV

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**Wednesday AM | October 20, 2021**  
**A120 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

**8:00 AM**

**Melt Pool Characterization and Numerical Simulation in Selective Laser Melting of NiTi Powder:** Stanislav Chernyshikhin<sup>1</sup>; Igor Shishkovsky<sup>1</sup>; <sup>1</sup>Skolkovo Institute of Science and Technology



# Technical Program

8:20 AM

**Additive Manufacturing of Titanium – Boron Carbide In Situ Composites:** *Mohan Sai Kiran Nartu<sup>1</sup>; Srinivas Aditya Mantri<sup>1</sup>; Thomas Scharf<sup>1</sup>; Brandon Mc Williams<sup>2</sup>; Kyu Cho<sup>2</sup>; Narendra Dahotre<sup>1</sup>; Rajarshi Banerjee<sup>1</sup>*; <sup>1</sup>University of North Texas; <sup>2</sup>CCDC U.S. Army Research Laboratory

8:40 AM

**Comparison of Mechanical Properties for Ti-Ta Vertically and Horizontally Graded Interfaces in Laser Powder Bed Fusion:** *Cherish Lesko<sup>1</sup>; Joseph Walker<sup>2</sup>; John Middendorf<sup>2</sup>; Joy Gockel<sup>1</sup>*; <sup>1</sup>Wright State University; <sup>2</sup>Arctos Technology Solutions

9:00 AM

**Multi-scale Strain, Microstructure, and Solidification Behavior of Ti-5553 Architected Lattice Melt Pools:** *Caleb Andrews<sup>1</sup>; Maria Strantza<sup>2</sup>; Tae Wook Heo<sup>2</sup>; Nicholas Calta<sup>2</sup>; Rongpei Shi<sup>2</sup>; Manyalibo Matthews<sup>2</sup>; Mitra Taheri<sup>1</sup>*; <sup>1</sup>Johns Hopkins University; <sup>2</sup>Lawrence Livermore National Laboratory

9:20 AM

**Effects of Process Parameters on Fracture and Fatigue of High Deposition Rate Laser Hot Wire Processed CP-Ti Grade 2:** *Hannah Sims<sup>1</sup>; John Lewandowski<sup>1</sup>*; <sup>1</sup>Case Western Reserve University

9:40 AM

**Mechanical Properties as a Function of Material State for Additively Manufactured Ti-5Al-5V-5Mo-3Cr:** *Andrew Temple<sup>1</sup>*; Madison Harrington<sup>1</sup>; Peter Collins<sup>1</sup>; <sup>1</sup>Iowa State University

10:00 AM

**Performance of Titanium Alloy Lattice Structures in Quasi-static and High Strain Rate Environments:** *John Carpenter<sup>1</sup>; Ben Brown<sup>2</sup>; Nathan Johnson<sup>3</sup>; Don Brown<sup>1</sup>; David Jones<sup>1</sup>; Borys Drach<sup>4</sup>; Jonathan Pegues<sup>5</sup>; Manyalibo Matthews<sup>6</sup>*; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Kansas City National Security Campus; <sup>3</sup>SLAC National Accelerator Laboratory; <sup>4</sup>New Mexico State University; <sup>5</sup>Sandia National Laboratories; <sup>6</sup>Lawrence Livermore National Laboratory

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## ENERGY

### Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments — Data Intensive and Correlative Methods

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Wednesday AM | October 20, 2021**

**A215 | Greater Columbus Convention Center**

**Session Chairs:** Janelle Wharry, Purdue University; Kevin Field, University of Michigan

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8:00 AM Invited

**Correlated Scattering and Microscopy Techniques for In-situ and Ex-situ Rapid Clustering Determination in Activated Materials:** *Kevin Field<sup>1</sup>; Samuel Briggs<sup>2</sup>; Caleb Massey<sup>3</sup>; Dalong Zhang<sup>4</sup>; Kenneth Littrell<sup>3</sup>*; <sup>1</sup>University of Michigan; <sup>2</sup>Oregon State University; <sup>3</sup>Oak Ridge National Laboratory; <sup>4</sup>Pacific Northwest National Laboratory

8:20 AM Invited

**Imaging Nanostructural Heterogeneities and Vacancy Supersaturation in Ni-20Cr after Corrosion in Molten Salt:** *Yang Yang<sup>1</sup>; Weiyue Zhou<sup>2</sup>; Shen Yin<sup>3</sup>; Sarah Wang<sup>4</sup>; Qin Yu<sup>3</sup>; Matthew J. Olszta<sup>5</sup>; Daniel K. Schreiber<sup>6</sup>; Jim Ciston<sup>3</sup>; Robert O. Ritchie<sup>3</sup>; Mark Asta<sup>3</sup>; Ju Li<sup>2</sup>; Michael P. Short<sup>2</sup>; Andrew M. Minor<sup>3</sup>*; <sup>1</sup>Pennsylvania State University; <sup>2</sup>MIT; <sup>3</sup>Lawrence Berkeley National Laboratory; <sup>4</sup>UCB; <sup>5</sup>PNNL

8:40 AM

**Multi-scale Characterization of Silicon Carbide Oxidation:** *Adam Bratten<sup>1</sup>; Haiming Wen<sup>1</sup>; Visharad Jalan<sup>1</sup>*; <sup>1</sup>Missouri University of Science and Technology

9:00 AM

**Europa Lander Contamination Control: Materials Testing and Numerical Simulation in a Flight Like Environment:** *Anthony Wong<sup>1</sup>*; <sup>1</sup>Jet Propulsion Lab, California Institute of Technology

9:20 AM

**A Closer Observation to the Precipitation Behavior of Proton Irradiated Dual Phase 308L Weldment Filler Materials:** *Zhen Li<sup>1</sup>; Xun Zhan<sup>1</sup>; Weicheng Zhong<sup>1</sup>; Benjamin Sutton<sup>2</sup>; Brent Heuser<sup>1</sup>*; <sup>1</sup>University of Illinois at Urbana-Champaign; <sup>2</sup>Electric Power Research Institute

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Session III

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**Wednesday AM | October 20, 2021**  
**A223 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

**8:00 AM**

**Towards a Fundamental Understanding of Surface Interactions and Degradation Mechanism in Bio-feedstock-induced Corrosion:** *Soheil Daryadel<sup>1</sup>; Deborah Liu<sup>1</sup>; Hyosung An<sup>1</sup>; Samyukta Shrivastava<sup>1</sup>; Siddhesh Shevade<sup>2</sup>; Tom Eason<sup>2</sup>; Qian Chen<sup>1</sup>; Daniel Krogstad<sup>1</sup>; Jessica Krogstad<sup>1</sup>*  
<sup>1</sup>University of Illinois at Urbana-Champaign; <sup>2</sup>BP

**8:20 AM**

**High-temperature Stability and Phase Transformations of Titanium Carbide (Ti3C2Tx) MXene:** *Srinivasa Kartik Neman<sup>1</sup>; Brian Wyatt<sup>1</sup>; Bowen Zhang<sup>1</sup>; Babak Anasori<sup>1</sup>*  
<sup>1</sup>Integrated Nanosystems Development Institute (INDI), IUPUI

**8:40 AM**

**Oxidation Behavior of IN100 Superalloy between 840 - 1120 K:** *Sebastian Lech<sup>1</sup>; Agnieszka Wusatowska-Sarne<sup>2</sup>; Adam Kruk<sup>1</sup>*  
<sup>1</sup>AGH University of Science and Technology; <sup>2</sup>Pratt & Whitney

## PROCESSING AND MANUFACTURING

### Advances in Surface Engineering — Advances in Surface Engineering

**Sponsored by:** TMS Surface Engineering Committee

**Program Organizers:** Rajeswaran Radhakrishnan, Faraday Technology Inc.; Brian Skinn, Faraday Technology, Inc.; Timothy Hall, Faraday Technology Inc.; Michael Roach, University of Mississippi Medical Center; Sandip Harimkar, Oklahoma State University; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University

**Wednesday AM | October 20, 2021**  
**A214 | Greater Columbus Convention Center**

**Session Chairs:** Rajeswaran Radhakrishnan, Faraday Technology, Inc.; Andrew Moran, Faraday Technology, Inc.

**8:00 AM**

**Engineering of Wearproof Surface by Management of Mechanical-Chemical Phenomena in Zone Contact:** *Volodymyr Tsyganov<sup>1</sup>; Richard Mokhnach<sup>1</sup>*  
<sup>1</sup>"Zaporizhzhia Polytechnic" National University

**8:20 AM**

**Methodological Principles of Engineering Surface Stainless Steel at Treatment Cutting with a Polymer:** *Volodymyr Tsyganov<sup>1</sup>; Sergey Sheyko<sup>2</sup>*  
<sup>1</sup>"Zaporizhzhia Polytechnic" National University; <sup>2</sup>Zaporizhzhia National University

**8:40 AM**

**Non-linear Through-hole Fabrication by Electrochemical Machining:** *Andrew Moran<sup>1</sup>; Brian Skinn<sup>1</sup>; Tim Hall<sup>1</sup>; Stephen Snyder<sup>1</sup>; Michael Horonzy<sup>2</sup>; Victor Alderman<sup>1</sup>*  
<sup>1</sup>Faraday Technology Inc.; <sup>2</sup>Republic Anode Fabricators

## CERAMIC AND GLASS MATERIALS

### Ceramics and Glasses Modeling by Simulations and Machine Learning — Session I

**Sponsored by:** ACerS Glass & Optical Materials Division

**Program Organizers:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**Wednesday AM | October 20, 2021**  
**B231 | Greater Columbus Convention Center**

**Session Chairs:** Mathieu Bauchy, UCLA; Peter Kroll, UT Arlington; Anoop Krishnan, IIT Delhi

**10:00 AM**

**Information Extraction Pipeline for Glasses: An NLP Based Approach:** *Vineeth Venugopal<sup>1</sup>; Sourav Sahoo<sup>1</sup>; Mohd Zaki<sup>1</sup>; Nitya Nand Goswami<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>*  
<sup>1</sup>IIT DELHI

**10:20 AM**

**A Machine-learning Based Hierarchical Framework to Discover Novel Scintillator Chemistries:** *Anjana Talapatra<sup>1</sup>; Blas Ueberuaga<sup>1</sup>; Christopher Stanek<sup>1</sup>; Ghanshyam Pilania<sup>1</sup>*  
<sup>1</sup>Los Alamos National Laboratory

**11:00 AM**

**The Energy Landscape Governs Ductility in Disordered Materials:** *Mathieu Bauchy<sup>1</sup>*  
<sup>1</sup>University of California, Los Angeles

**10:40 AM**

**Kinetic Monte Carlo Simulation of Glasses Aided by Machine Learning:** *Ajay Annamareddy<sup>1</sup>*  
<sup>1</sup>University of Wisconsin - Madison

## MATERIALS-ENVIRONMENT INTERACTIONS

### Computation Assisted Materials Development for Improved Corrosion Resistance — A: Low Temperature Corrosion

**Program Organizers:** Rishi Pillai, Oak Ridge National Laboratory; Laurence Marks, Northwestern University

**Wednesday AM | October 20, 2021**  
**A222 | Greater Columbus Convention Center**

**Session Chair:** David Shifler, Office of Naval Research

**8:00 AM** Introductory Comments

**8:05 AM** Invited

**Factors That Influence Materials Corrosion and How Modeling May Predict These Effects:** *David Shifler<sup>1</sup>*  
<sup>1</sup>Office of Naval Research

# Technical Program

8:35 AM

**Back to the Basics: Revisiting Copper to Build Thermodynamic Corrosion Models:** *Lauren Walters*<sup>1</sup>; Liang-Feng Huang<sup>2</sup>; James Rondinelli<sup>1</sup>; <sup>1</sup>Northwestern University; <sup>2</sup>Ningbo Institute of Materials Technology and Engineering

8:55 AM

**Computational Modeling of Corrosion and Mechanical Failure in Magnesium-Aluminum Vehicle Joints:** *Kubra Karayagiz*<sup>1</sup>; Adam Powell<sup>1</sup>; Qingli Ding<sup>1</sup>; Brajendra Mishra<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

9:15 AM

**Development of a Damage Function for Galvanic Corrosion Degradation of Coated Al Alloy Systems:** *Mahdi Jokar*<sup>1</sup>; Gerald Frankel<sup>1</sup>; <sup>1</sup>Ohio State University

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## NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — Nanoparticles & Nanocomposites I

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

Wednesday AM | October 20, 2021

B240/241 | Greater Columbus Convention Center

**Session Chairs:** Edward Gorzkowski, Naval Research Laboratory; Kathy Lu, Virginia Tech

8:00 AM Invited

**Controlling Grain Growth with Anisotropic Interfacial Energy and Heterogeneous Segregation:** *Amanda Krause*<sup>1</sup>; <sup>1</sup>University of Florida

8:30 AM

**Low Temperature Synthesis of Metastable Tetragonal Yttria Doped Hafnia T-(Y-HfO<sub>2</sub>) Nanoparticles Through Mechanochemical Processing and Annealing:** *Zanlin Qiu*<sup>1</sup>; Cheng-han Li<sup>1</sup>; Joerg Jinschek<sup>1</sup>; Pelagia-Irene (Perena) Gouma<sup>1</sup>; <sup>1</sup>Ohio State University

8:50 AM Invited

**Design of Nanoparticles from Environmentally Benign Precursors:** *Surojit Gupta*<sup>1</sup>; <sup>1</sup>University of North Dakota

9:20 AM

**Surface Oxidation Behavior of FeNi-based Metal Amorphous Nanocomposite (MANC) for High Speed Motor Applications:** *James Egbu*<sup>1</sup>; Paul Ohodnicki<sup>2</sup>; Ruishu Wright<sup>3</sup>; John Baltrus<sup>3</sup>; Michael McHenry<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>University of Pittsburgh; <sup>3</sup>National Energy Technology Laboratory

9:40 AM

**Mechanisms of Hillock Formation and Nanostructural Self-assembly during Vapor-deposition of Phase-separating Alloy Films:** *Rahul Raghavan*<sup>1</sup>; *Kumar Ankit*<sup>1</sup>; <sup>1</sup>Arizona State University

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## ENERGY

### Energy Materials for Sustainable Development — Fuel Cells / Storage Batteries II

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

Wednesday AM | October 20, 2021

A216 | Greater Columbus Convention Center

**Session Chairs:** Julia Zaikina, Iowa State University; Mona Zebbarjadi, University of Virginia

8:00 AM

**Magnesium-air Fuel Cell and MgO Electrolyzer:** *Hongyi Sun*<sup>1</sup>; Armaghan Telgerafchi<sup>2</sup>; Madison Rutherford<sup>2</sup>; Gabriel Espinosa<sup>2</sup>; Lucien Wallace<sup>2</sup>; Adam Powell<sup>2</sup>; *Mahya Shahabi*<sup>2</sup>; <sup>1</sup>University of Maryland, College Park; <sup>2</sup>Worcester Polytechnic Institute

8:20 AM

**Improving Intermediate-temperature Solid Oxide Fuel Cell Anode Performance with Metal and MIEC Nanocatalyst Infiltration:** *Jillian Rix*<sup>1</sup>; Boshan Mo<sup>1</sup>; Uday Pal<sup>1</sup>; Srikanth Gopalan<sup>1</sup>; Soumendra Basu<sup>1</sup>; <sup>1</sup>Boston University

8:40 AM

**Liquid Metal Anode Direct Carbon Fuel Cell:** *Steven Jacek*<sup>1</sup>; Christian Faria<sup>1</sup>; Adam Powell<sup>1</sup>; Boyd Davis<sup>2</sup>; Yu Zhong<sup>1</sup>; Uday Pal<sup>3</sup>; Soumendra Basu<sup>3</sup>; <sup>1</sup>Worcester Polytechnic Institute; <sup>2</sup>Kingston Process Metallurgy; <sup>3</sup>Boston University

9:00 AM Invited

**The Role of Lithium Site Occupancy on Lithium-Ion Conductivity of Tantalum-Doped Lithium Lanthanum Zirconium Oxide Garnet:** *Jeffrey Fergus*<sup>1</sup>; Xingxing Zhang<sup>1</sup>; <sup>1</sup>Auburn University

9:30 AM

**One-step Synthesis of Carbon-coated LiCoPO<sub>4</sub> Nanopowders for High Voltage Battery Cathodes:** *V. V. Rohit Bukka*<sup>1</sup>; Pankaj Sarin<sup>1</sup>; <sup>1</sup>Oklahoma State University

## IRON AND STEEL (FERROUS ALLOYS)

### Fracture of Steels: New Approaches to Modeling and Experimental Characterization — Session I

**Sponsored by:** TMS Steels Committee

**Program Organizers:** Louis Hector, General Motors Global Technical Center; Ana Luiza Araujo, AK Steel Research & Innovation; Matthias Militzer, University of British Columbia; Amy Clarke, Colorado School of Mines

**Wednesday AM | October 20, 2021**  
**A211 | Greater Columbus Convention Center**

**Session Chair:** Ana Araujo, CBMM

**8:00 AM**

**Applied Potential Influence on Stress Corrosion Cracking Susceptibility of 316LN Stainless Steel Rebars in Simulated Concrete Pore Solution with Chlorides:** *Ulises Martin*<sup>1</sup>; Jacob Rössl<sup>1</sup>; Juan Bosch<sup>1</sup>; David M. Bastidas<sup>1</sup>; <sup>1</sup>University of Akron

**8:20 AM Invited**

**Fracture Anisotropy of SS-304L Tubes under Biaxial Loading:** Madhav Baral<sup>1</sup>; Yannis Korkolis<sup>2</sup>; <sup>1</sup>University of New Hampshire; <sup>2</sup>The Ohio State University

**8:50 AM**

**Local Micromechanical Properties of Inclusions in Ferrous Alloys:** Alejandra Slagter<sup>1</sup>; Joris Everaerts<sup>1</sup>; Léa Deillon<sup>1</sup>; *Andreas Mortensen*<sup>1</sup>; <sup>1</sup>EPFL

**9:10 AM Keynote**

**The Mechanics of Size Effect in Brittle Fracture of Steel: Connecting the Change in Strain Energy and Its Planar Dissipation to Rationalize the Size-effect:** *K. S. Ravi Chandran*<sup>1</sup>; <sup>1</sup>University of Utah

**9:50 AM**

**Peculiarities of Mechanics Destruction Tribojoints at a Difficult Dynamic Loading:** *Volodymyr Tsyganyov*<sup>1</sup>; Sergey Sheyko<sup>2</sup>; <sup>1</sup>Zaporizhzhia Polytechnic National University; <sup>2</sup>Zaporizhzhia National University

## ELECTRONIC AND MAGNETIC MATERIALS

### Functional Defects in Electroceramic Materials — Session I: Defect Engineering in Ceramic Materials

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Hui Xiong, Boise State University; Hua Zhou, Argonne National Laboratory

**Wednesday AM | October 20, 2021**  
**B235 | Greater Columbus Convention Center**

**Session Chairs:** Claire Xiong, Boise State University; Hua Zhou, Argonne National Lab

**10:00 AM Introductory Comments**

**10:05 AM Invited**

**Let Thermodynamics do Interfacial Engineering:** *Jian Luo*<sup>1</sup>; <sup>1</sup>University of California, San Diego

**10:45 AM Invited**

**Accelerated Synthesis and In-situ X-ray Pair Distribution Functions of Substituted Vanadium Dioxide:** *Vicky Doan-Nguyen*<sup>1</sup>; <sup>1</sup>Ohio State University

**11:15 AM Invited**

**Understanding Lithium Plating in Graphite and Silicon for Fast Charging Li-ion Battery:** *Tao Gao*<sup>1</sup>; <sup>1</sup>University of Utah

## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Processing and Properties II

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Wednesday AM | October 20, 2021**  
**B131 | Greater Columbus Convention Center**

**Session Chairs:** Fei Wang, University of Nebraska Lincoln; Chanho Lee, Los Alamos National Laboratory

**8:00 AM**

**Irradiation Damage in (Zr<sub>0.25</sub>Ta<sub>0.25</sub>Nb<sub>0.25</sub>Ti<sub>0.25</sub>)C High-entropy Carbide Ceramics:** *Fei Wang*<sup>1</sup>; Xueliang Yan<sup>1</sup>; Tianyao Wang<sup>2</sup>; Yaqiao Wu<sup>3</sup>; Lin Shao<sup>2</sup>; Michael Nastasi<sup>2</sup>; Yongfeng Lu<sup>1</sup>; Bai Cui<sup>1</sup>; <sup>1</sup>University of Nebraska Lincoln; <sup>2</sup>Texas A&M University; <sup>3</sup>Boise State University

**8:20 AM Invited**

**Radiation Effects in High Entropy Alloys:** *Shradha Agarwal*<sup>1</sup>; Steven Zinkle<sup>1</sup>; <sup>1</sup>University of Tennessee



# Technical Program

8:40 AM

**Stress-corrosion of Al<sub>0.1</sub>CoCrFeNi High Entropy Alloy in a Molten Eutectic Salt:** Xinyi Wang<sup>1</sup>; Madison McGrann<sup>1</sup>; James Earthman<sup>1</sup>; <sup>1</sup>University of California-Irvine

9:00 AM

**Amorphous Bands Induced by Low Temperature Tension in a Non-equiatomical CrMnFeCoNi Alloy:** Jian Wang<sup>1</sup>; Kaisheng Ming<sup>2</sup>; <sup>1</sup>University of Nebraska-Lincoln; <sup>2</sup>Hebei University of Technology

9:20 AM Invited

**Using Large Scale Ab Initio Computing to Predict and Understand High Entropy Alloys Formation:** Geoffroy Hautier<sup>1</sup>; G.B. Bokas<sup>2</sup>; W. Chen<sup>2</sup>; Stephane Gorsse<sup>3</sup>; A. Hilhorst<sup>2</sup>; P. Jacques<sup>2</sup>; <sup>1</sup>UCLouvain; Dartmouth College; <sup>2</sup>UCLouvain; <sup>3</sup>ICMB

9:50 AM

**The Formation of Complex Ternary Oxides in Refractory Complex Concentrated Alloys:** Logan Ware<sup>1</sup>; Brahim Akdim<sup>2</sup>; Christopher Woodward<sup>3</sup>; Tinuade Daboiku<sup>2</sup>; Todd Butler<sup>3</sup>; Oleg Senkov<sup>2</sup>; Samuel Kuhr<sup>3</sup>; Noah Philips<sup>4</sup>; Michael Titus<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>UES Inc.; <sup>3</sup>Air Force Research Laboratory; <sup>4</sup>ATI Specialty Alloys and Components

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## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Theory and Modeling I

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Wednesday AM | October 20, 2021**

**B132 | Greater Columbus Convention Center**

**Session Chairs:** Dilpuneet Aidhy, University of Wyoming; Yong-Jie Hu, Drexel University

8:00 AM Invited

**Data-enabled Additive Manufacturing of High-entropy Alloys:** Ganesh Balasubramanian<sup>1</sup>; Praveen Sreeramagiri<sup>1</sup>; <sup>1</sup>Lehigh University

8:30 AM Invited

**Data-driven Design of Refractory High-entropy Alloys:** George Kim<sup>1</sup>; Chanhoo Lee<sup>2</sup>; Peter Liaw<sup>3</sup>; Wei Chen<sup>1</sup>; <sup>1</sup>Illinois Institute of Technology; <sup>2</sup>Los Alamos National Lab; <sup>3</sup>University of Tennessee

8:50 AM

**A Systematic Analysis of Phase Stability in Refractory High Entropy Alloys Utilizing Linear and Non-linear Cluster Expansion Models:** Chiraag Nataraj<sup>1</sup>; Edgar Josué Landinez Borda<sup>2</sup>; Axel van de Walle<sup>1</sup>; Amit Samanta<sup>2</sup>; <sup>1</sup>Brown University; <sup>2</sup>Lawrence Livermore National Lab

9:10 AM Invited

**Atomic Transport by Point Defects and Clusters in Concentrated Alloys:** Osetskiy Yuriy<sup>1</sup>; Laurent Béland<sup>2</sup>; Alexander Barashev<sup>3</sup>; Yanwen Zhang<sup>4</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Queen's University; <sup>3</sup>University of Michigan; <sup>4</sup>University of Tennessee

9:30 AM Invited

**Joint Prediction of Mechanical Properties of Alloys with Enhanced Fidelity through Integration of Machine Learning (Data Analytics) and Multiscale Modeling:** Baldur Steingrimssohn<sup>1</sup>; Peter Liaw<sup>2</sup>; Jaafar El-Awady<sup>3</sup>; <sup>1</sup>Imagars LLC; <sup>2</sup>University of Tennessee; <sup>3</sup>John Hopkins University

9:50 AM Invited

**Predicting Fundamental Properties of BCC Refractory Multicomponent Alloys Using Electronic Descriptors and Statistical Learning:** Yong-Jie Hu<sup>1</sup>; Christopher Tandoc<sup>1</sup>; Liang Qi<sup>2</sup>; <sup>1</sup>Drexel University; <sup>2</sup>University of Michigan

10:20 AM Break

10:40 AM Invited

**Machine Learning Enabled Defect Energies in Concentrated Alloys:** Gaurav Arora<sup>1</sup>; Anus Manzoor<sup>1</sup>; Dilpuneet Aidhy<sup>1</sup>; <sup>1</sup>University of Wyoming

11:00 AM Invited

**Determination of Fluctuations in Local Composition, Strain and Lattice Distortions in Multi-principal Component Alloys Using Advanced Transmission Electron Microscopy:** Jian Min Zuo<sup>1</sup>; Haw-Wen Hsiao<sup>1</sup>; Yu-Tsun Shao<sup>1</sup>; Qun Yang<sup>1</sup>; Yang Hu<sup>1</sup>; <sup>1</sup>University of Illinois

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## CERAMIC AND GLASS MATERIALS

### Journal of the American Ceramic Society Awards Symposium — Journal of the American Ceramic Society Awards Symposium I

**Sponsored by:** ACerS

**Program Organizer:** William Fahrenholtz, Missouri University of Science and Technology

**Wednesday AM | October 20, 2021**

**B233 | Greater Columbus Convention Center**

**Session Chairs:** William Fahrenholtz, Missouri University of Science and Technology; Jonathon Foreman, American Ceramic Society

8:00 AM Introductory Comments

8:10 AM Invited

**A Novel Strategy to Strengthen Alumina-carbon Refractories for Flow Control of Molten Steel:** Zhe Chen<sup>1</sup>; Wen Yan<sup>1</sup>; Stefan Schafföner<sup>2</sup>; Yajie Dai<sup>1</sup>; Qiang Wang<sup>1</sup>; Guangqiang Li<sup>1</sup>; <sup>1</sup>Wuhan University of Science and Technology; <sup>2</sup>University of Bayreuth

8:40 AM Invited

**A Thermodynamics-guided Framework to Design Spherical Lightweight Aggregate from Waste Coal Combustion Ash:** Mohammad Balapour<sup>1</sup>; Thiha Thway<sup>1</sup>; Rathin Rao<sup>1</sup>; Newell Moser<sup>2</sup>; Edward Garboczi<sup>2</sup>; Yick Hsuan<sup>1</sup>; Sabrina Spataro<sup>1</sup>; Yaghoob Farnam<sup>1</sup>; <sup>1</sup>Drexel University; <sup>2</sup>National Institute of Standards and Technology

9:10 AM Invited

**Direct Ink Writing (DIW) of Hierarchical Porous Alumina Stabilized Emulsions: Rheology and Printability:** George Franks<sup>1</sup>; Shareen Chan<sup>1</sup>; Mitchell Sesso<sup>2</sup>; <sup>1</sup>University of Melbourne; <sup>2</sup>La Trobe University

9:40 AM Invited

**Effect of Moisture on the Oxidation Behaviour of ZrB<sub>2</sub>:** Ravisankar Naraparaju<sup>1</sup>; <sup>1</sup>German Aerospace Center

**10:10 AM Break**

**10:30 AM Invited**

**Processing of MAX Phases: From Synthesis to Applications:** *Jesus Gonzalez-Julian<sup>1</sup>; <sup>1</sup>Forschungszentrum Jülich*

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## CERAMIC AND GLASS MATERIALS

### Manufacturing and Processing of Advanced Ceramic Materials — Processing of Carbides, Borides, and Nitrides

**Sponsored by:** ACerS Manufacturing Division

**Program Organizers:** Bai Cui, University of Nebraska-Lincoln; James Hemrick, Oak Ridge National Laboratory; Mike Alexander, Allied Mineral Products; Eric Faierson, Quad City Manufacturing Laboratory/Western Illinois University; Keith DeCarlo, Blasch Precision Ceramics

**Wednesday AM | October 20, 2021**

**B234 | Greater Columbus Convention Center**

**Session Chairs:** Brian Leonard, University of Wyoming; Fei Wang, University of Nebraska-Lincoln

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**10:00 AM Invited**

**Low Temperature Synthesis Methods for Nanoparticle Carbides:** *Brian Leonard<sup>1</sup>; <sup>1</sup>University of Wyoming*

**10:40 AM**

**Bulk Amorphous SiCN Produced through Plasma Synthesis and Spark Plasma Sintering:** *Steven Herzberg<sup>1</sup>; Suveen Mathaudhu<sup>1</sup>; Lorenzo Mangolini<sup>1</sup>; <sup>1</sup>University of California, Riverside*

**11:00 AM**

**Development of New Synthesis Route for Environmentally Friendly Thermoelectric Rare Earth Borocarbonitrides for Upcoming Carbon-neutral Society:** *Hyoung-Won Son<sup>1</sup>; Takao Mori<sup>2</sup>; Masatoshi Takeda<sup>1</sup>; David Berthebaud<sup>2</sup>; Philipp Sauerschnig<sup>3</sup>; Quansheng Guo<sup>2</sup>; Tadachika Nakayama<sup>1</sup>; <sup>1</sup>Nagaoka University of Technology; <sup>2</sup>National Institute for Materials Science; <sup>3</sup>National Institute of Advanced Industrial Science and Technology*

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## ARTIFICIAL INTELLIGENCE

### Materials Informatics for Images and Multi-dimensional Datasets — Session I

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Amanda Krause, University of Florida; Alp Sehirlioglu, Case Western Reserve University; Daniel Ruscitto, General Electric

**Wednesday AM | October 20, 2021**

**A124 | Greater Columbus Convention Center**

**Session Chair:** Amanda Krause, University of Florida

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**8:00 AM Invited**

**Machine Learning and Image Processing Techniques for Materials Evaluation:** *Roger French<sup>1</sup>; Benjamin Pierce<sup>1</sup>; <sup>1</sup>Case Western Reserve University*

**8:30 AM**

**Quantitative Comparisons of 2D Microstructures with the Wasserstein Metric:** *Ethan Suwandi<sup>1</sup>; Jeremy Mason<sup>1</sup>; <sup>1</sup>University of California Davis*

**8:50 AM**

**Spatial and Statistical Representation of Strain Localization as a Function of the 3D Microstructure Using Multi-modal and Multi-scale Data Merging:** *Marie Charpagne<sup>1</sup>; J.C. Stinville<sup>1</sup>; Andrew T. Polonsky<sup>2</sup>; McLean P. Echlin<sup>1</sup>; Kelly Nygren<sup>3</sup>; Dalton Shadle<sup>3</sup>; Matthew P. Miller<sup>3</sup>; Tresa M. Pollock<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>Sandia National Laboratories; <sup>3</sup>Cornell University*

**9:10 AM**

**Building a Database of Fatigue Fracture Images to train a CNN:** *Katelyn Jones<sup>1</sup>; Paul Shade<sup>2</sup>; William Musinski<sup>2</sup>; Reji John<sup>2</sup>; Adam Pilchak<sup>2</sup>; Anthony Rollett<sup>1</sup>; Elizabeth Holm<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Air Force Research Laboratory*

# Technical Program

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## IRON AND STEEL (FERROUS ALLOYS)

### New Frontiers in Physical Metallurgy of Steels — New Frontiers in Physical Metallurgy of Steels I

**Sponsored by:** AIST: MPPA Committee, TMS Steels Committee

**Program Organizers:** Matthias Militzer, University of British Columbia; Pello Uranga, CEIT and TECNUN (University of Navarra); Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Amit Behera, QuesTek Innovations LLC

**Wednesday AM | October 20, 2021**  
**A210 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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#### 8:00 AM Invited

**Microstructural Engineering and Accelerated Test Method Development to Achieve Low Cost, High Performance Solutions for Hydrogen Storage and Delivery:** *Kip Findley*<sup>1</sup>; John Speer<sup>1</sup>; Lawrence Cho<sup>1</sup>; Pawan Kathayat<sup>1</sup>; Yuran Kong<sup>1</sup>; Chris San Marchi<sup>2</sup>; Brian Kagay<sup>2</sup>; Samantha Lawrence<sup>3</sup>; Joseph Ronevich<sup>2</sup>; Ashok Saxena<sup>4</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Sandia National Laboratory; <sup>3</sup>Los Alamos National Laboratory; <sup>4</sup>WireTough Cylinders

#### 8:40 AM

**Microstructural Modeling and Design in Triple Nano-precipitate Strengthened Austenitic Steel:** *Colin Stewart*<sup>1</sup>; Richard Fonda<sup>2</sup>; Keith Knipling<sup>2</sup>; Patrick Callahan<sup>2</sup>; <sup>1</sup>NRC Associate at the US Naval Research Laboratory; <sup>2</sup>US Naval Research Laboratory

#### 9:10 AM

**Improving the Fatigue Performance of Nitrided Steels with Amorphous and Crystalline Precipitates:** *Jonah Klemm-Toole*<sup>1</sup>; Kip Findley<sup>1</sup>; <sup>1</sup>Colorado School of Mines

#### 9:40 AM

**Obtaining High Strength Ductility Combination by Quenching and Partitioning of Rolled Low Carbon Steel Sheet:** *Alok Singh*<sup>1</sup>; Basudev Bhattacharya<sup>2</sup>; Somjeet Biswas<sup>3</sup>; <sup>1</sup>Indian Institute of Technology Kharagpur; <sup>2</sup>Tata Steel Limited, India; <sup>3</sup>IIT Kharagpur

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## BIOMATERIALS

### Next Generation Biomaterials — Session III

**Sponsored by:** ACerS Bioceramics Division, TMS Biomaterials Committee

**Program Organizers:** Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

**Wednesday AM | October 20, 2021**  
**A224 | Greater Columbus Convention Center**

**Session Chairs:** Emiyl Lazarus, Rochester Institute of Technology; Hamdy Ibrahim, University of Tennessee Chattanooga; Sandra Musu Jusu, Worcester Polytechnic Institute

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#### 8:00 AM

**Comparison of Various Post Coating Treatments on Plasma Sprayed HA Coatings:** *Manoj Mittal*<sup>1</sup>; *Tarun Goyal*<sup>1</sup>; <sup>1</sup>IK Gujral Punjab Technical University Jalandhar

#### 8:20 AM

**Corrosion Assessment of Rare Earth Elements and Magnesium-based Nanocomposites for Bio-implant Applications:** *Moataz Abdalla*<sup>1</sup>; *Austin Sims*<sup>1</sup>; *Meysam Haghshenas*<sup>2</sup>; *Manoj Gupta*<sup>3</sup>; *Hamdy Ibrahim*<sup>1</sup>; <sup>1</sup>University of Tennessee at Chattanooga; <sup>2</sup>University of Toledo; <sup>3</sup>National University of Singapore

#### 8:40 AM Invited

**Hierarchical Hybrid Carbon Nanotube Enhanced Bioscaffolds for Wound Healing:** *Soham Parikh*<sup>1</sup>; *Wenhu Wang*<sup>2</sup>; *Tyler Nelson*<sup>3</sup>; *Courtney Sulentic*<sup>1</sup>; *Sharmila Mukhopadhyay*<sup>2</sup>; <sup>1</sup>Wright State University; <sup>2</sup>The University of Maine; <sup>3</sup>Wright-Patterson Air Force Base

#### 9:00 AM

**In Vivo And In Vitro Evaluation of PLGA-PEG Microspheres Loaded with LHRH-Targeted Drugs for Effective Breast Cancer Treatment:** *Sandra Jusu*<sup>1</sup>; *John Obayemi*<sup>1</sup>; *Ali Salifu*<sup>1</sup>; *Chukwudalu Nwazojie*<sup>2</sup>; *Vanessa Uzonwanne*<sup>1</sup>; *Olushola Odusanya*<sup>3</sup>; *Winston Soboyejo*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute; <sup>2</sup>African University of Science and Technology; <sup>3</sup>Sheda Science and Technology Complex (SHESTCO)

#### 9:20 AM

**Innovative Solutions to Produce Bioceramic Implants by 3D Printing:** *Kenna Ritter*<sup>1</sup>; *Peter Durcan*<sup>1</sup>; <sup>1</sup>3DCERAM SINTO INC

#### 9:40 AM

**Synthesis of Three-dimensional Ceramic Microlattices by Aerosol Jet Nanoparticle Printing and their Use in Cancer Biomarker Detection:** *Bin Yuan*<sup>1</sup>; *Chunshan Hu*<sup>1</sup>; *Azahar Ali*<sup>1</sup>; *Rahul Panat*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

## CERAMIC AND GLASS MATERIALS

### Preceramic Polymers; Synthesis, Processing, Modeling, and Derived Ceramics — Preceramic Polymers and Polymer Derived Ceramics I

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Matthew Dickerson, Air Force Research Laboratory; Gurpreet Singh, Kansas State University; Paolo Colombo, University of Padova; Günter Motz, Universität Bayreuth

**Wednesday AM | October 20, 2021**  
**B230 | Greater Columbus Convention Center**

**Session Chair:** Matthew Dickerson, Air Force Research Laboratory

#### 8:00 AM Introductory Comments Organizers' Remarks

##### 8:10 AM Invited

**UV Curable Preceramic Polymers and their Application in Additive Manufacturing:** Tobias Schaedler<sup>1</sup>; Kayleigh Porter<sup>1</sup>; Mark O'Masta<sup>1</sup>; Ekaterina Stonkevitch<sup>1</sup>; Zak Eckel<sup>1</sup>; Phuong Bui<sup>1</sup>; <sup>1</sup>HRL Laboratories LLC

##### 8:40 AM

**Preparation of ZrC-embedded Glass-like Carbon Wires via Thermal Decomposition of Metal Organic Frameworks:** Kaitlyn Shirey<sup>1</sup>; Brittany Bonnett<sup>2</sup>; Xiaozhou Yang<sup>2</sup>; Amanda Morris<sup>2</sup>; Carolina Tallon<sup>2</sup>; <sup>1</sup>Virginia Polytechnic Institute; <sup>2</sup>Virginia Tech

##### 9:00 AM

**X-ray Computed Tomography Investigation of CMC Densification via Polymer Infiltration and Pyrolysis:** Derek King<sup>1</sup>; Thomas Key<sup>1</sup>; Connor Wycoff<sup>1</sup>; Craig Przybyla<sup>2</sup>; Michael Cinibulk<sup>2</sup>; <sup>1</sup>UES Inc; <sup>2</sup>AFRL

## FUNDAMENTALS AND CHARACTERIZATION

### Probing Defect Properties and Behavior under Mechanical Deformation and Extreme Conditions — Radiation Response and Defect Evolution

**Sponsored by:** TMS Nanomechanical Materials Behavior Committee, TMS Nuclear Materials Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Zhe Fan, Lamar University; Tianyi Chen, Oregon State University; Shijun Zhao, City University of Hong Kong; Mitra Taheri, Johns Hopkins University; Yury Osetskiy, Oak Ridge National Laboratory

**Wednesday AM | October 20, 2021**  
**B140/141 | Greater Columbus Convention Center**

**Session Chairs:** Xing Wang, Pennsylvania State University; Tianyi Chen, Oregon State University

##### 8:00 AM Invited

**Radiation Enhanced Diffusion in Fe2O3 and Cr2O3:** Kayla Yano<sup>1</sup>; Aaron Kohnert<sup>2</sup>; Amitava Banerjee<sup>2</sup>; Danny Edwards<sup>1</sup>; Edward Holby<sup>2</sup>; Tiffany Kaspar<sup>1</sup>; Hyosim Kim<sup>2</sup>; Sandra Taylor<sup>1</sup>; Yongqiang Wang<sup>2</sup>; Blas Uberuaga<sup>2</sup>; Daniel Schreiber<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Los Alamos National Laboratory

##### 8:30 AM

**Impact of Grain Boundary and Surface Diffusion on Fission Gas Release in UO<sub>2</sub> Nuclear Fuel Using a Phase Field Model:** Md Ali Muntaha<sup>1</sup>; Dong-Uk Kim<sup>1</sup>; Michael Tonks<sup>1</sup>; <sup>1</sup>University of Florida

##### 8:50 AM Invited

**Long-range One-dimensional Glide of Defect Clusters in Irradiated Materials: Experimental Evidence and Consequences:** Steven Zinkle<sup>1</sup>; Ling Wang<sup>2</sup>; Yan-Ru Lin<sup>1</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Oak Ridge National Lab

##### 9:20 AM Invited

**The Role of Anisotropy on the Defect Self-organization in Metals under Irradiation:** Cheng Sun<sup>1</sup>; <sup>1</sup>Idaho National Laboratory

##### 9:50 AM Invited

**Surprisingly High Irradiation-induced Defect Mobility in Fe3O4 as Revealed through In Situ Transmission Electron Microscopy:** Djamel Kaoum<sup>1</sup>; Martin Owusu-Mensah<sup>1</sup>; Angelica Lopez Morales<sup>1</sup>; Kayla Yano<sup>2</sup>; Tiffany Kaspar<sup>2</sup>; Daniel Schreiber<sup>2</sup>; Blas Uberuaga<sup>3</sup>; <sup>1</sup>North Carolina State University; <sup>2</sup>Pacific Northwest National Laboratory; <sup>3</sup>Los Alamos National Laboratory

##### 10:20 AM Break

##### 10:40 AM Invited

**Multimodal and Multiscale Defect Characterization and Property Correlation for Nuclear Fuel and Materials via Advanced Post Irradiation Examination Techniques:** Peng Xu<sup>1</sup>; <sup>1</sup>Idaho National Laboratory

##### 11:10 AM

**Measuring Elemental Segregation and Vacancy Migration Using Atom Probe Tomography:** Xing Wang<sup>1</sup>; Jonathan Poplawsky<sup>2</sup>; Yanwen Zhang<sup>3</sup>; Karren More<sup>2</sup>; <sup>1</sup>Pennsylvania State University; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>University of Tennessee

## FUNDAMENTALS AND CHARACTERIZATION

### Processing—Microstructure—Property Relationships of Titanium and Titanium Alloys — Session I

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Yufeng Zheng, University of Nevada-Reno; Rongpei Shi, Lawrence Livermore National Laboratory; Michael Gram, Titanium Metals Corporation

**Wednesday AM | October 20, 2021**  
**B246 | Greater Columbus Convention Center**

**Session Chairs:** Yufeng Zheng, University of Nevada Reno; Rongpei Shi, Lawrence Livermore National Laboratory

##### 8:00 AM Invited

**Exploiting Structural and Compositional Instabilities in Titanium Alloys to Optimize Microstructure/Property Interrelationships in Samples Fabricated by Additive Manufacturing:** Brian Welk<sup>1</sup>; Nevin Taylor<sup>1</sup>; Zachary Kloenne<sup>1</sup>; Yufeng Zheng<sup>2</sup>; Rajarshi Banerjee<sup>3</sup>; Hamish Fraser<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>University of Nevada-Reno; <sup>3</sup>University of North Texas

##### 8:30 AM Invited

**Regulating Elastic and Plastic Deformation by Heterogeneous Microstructure Design in Ti-alloys:** Yunzhi Wang<sup>1</sup>; <sup>1</sup>Ohio State University



# Technical Program

9:00 AM Invited

**Influence of Athermal vs. Isothermal Omega Precipitation and Alpha Precipitation on TRIP/TWIP Deformation Mechanisms in Metastable Beta Ti alloys (invited):** Srinivas Aditya Mantri<sup>1</sup>; Abhishek Sharma<sup>1</sup>; Riyadh Salloom<sup>1</sup>; MSKKY Nartu<sup>1</sup>; Sriswaroop Dasari<sup>1</sup>; Srinivasan Srivilliputhur<sup>1</sup>; *Rajarshi Banerjee*<sup>1</sup>; <sup>1</sup>University of North Texas

9:30 AM

**Nano-scale O" Phase and Fine-scale Alpha Precipitation in a Metastable Beta Ti-5Al-5Mo-5V-3Cr Alloy:** Dian Li<sup>1</sup>; Stoichko Antonov<sup>2</sup>; Rongpei Shi<sup>3</sup>; Zachary Kloenne<sup>4</sup>; Hamish Fraser<sup>4</sup>; *Yufeng Zheng*<sup>5</sup>; <sup>1</sup>University of Nevada-Reno; <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH; <sup>3</sup>Lawrence Livermore National Laboratory; <sup>4</sup>Ohio State University; <sup>5</sup>University of Nevada-Reno

9:50 AM

**A Data-driven Analysis for Selection and Use of Conventional Ti Alloys for Aeroengine Applications and Future Directions:** *Tanjore Jayaraman*<sup>1</sup>; Ramachandra Canumalla<sup>2</sup>; <sup>1</sup>University of Michigan-Dearborn; <sup>2</sup>Weldaloy Specialty Forgings

10:10 AM Break

10:30 AM

**The BMG to Ti Weld, a Pool for Microstructure: Property Characterization:** Dan Sorensen<sup>1</sup>; Eric Hintsala<sup>2</sup>; Jesse Pischlar<sup>3</sup>; Joseph Stevick<sup>4</sup>; Bernie Li<sup>3</sup>; Daniel Kiener<sup>5</sup>; Jason Meyers<sup>6</sup>; Antonio Ramirez<sup>7</sup>; *Douglas Stauffer*<sup>2</sup>; Robert Ritchie<sup>8</sup>; <sup>1</sup>Boston Scientific; <sup>2</sup>Bruker Nano Surfaces & Metrology; <sup>3</sup>Medtronic; <sup>4</sup>Hummingbird Scientific; <sup>5</sup>Montanuniversität, Leoben; <sup>6</sup>University of Minnesota; <sup>7</sup>Ohio State University; <sup>8</sup>University of California, Berkeley

10:50 AM

**Role of Novel Highly-indexed Twinning in Hierarchical a Microstructure in Metastable  $\beta$  Ti-5Al-5Mo-5V-3Cr Alloy:** *Dian Li*<sup>1</sup>; Wenrui Zhao<sup>1</sup>; Xing Zhang<sup>2</sup>; Stoichko Antonov<sup>3</sup>; Yiliang Liao<sup>2</sup>; Yufeng Zheng<sup>1</sup>; <sup>1</sup>University of Nevada, Reno; <sup>2</sup>Iowa State University; <sup>3</sup>Max-Planck-Institut für Eisenforschung GmbH

11:10 AM

**The Composition-processing-microstructure-property Relationships of Fe and Al Modified Ti-Cr Alloys:** *Joann Ballor*<sup>1</sup>; Jonathan Poplawsky<sup>2</sup>; Elizabeth Kautz<sup>3</sup>; Bharat Gwalani<sup>3</sup>; Arun Devaraj<sup>3</sup>; Masahiko Ikeda<sup>4</sup>; Carl Boehlert<sup>1</sup>; <sup>1</sup>Michigan State University; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>Pacific Northwest National Laboratory; <sup>4</sup>Kansai University

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## MATERIALS-ENVIRONMENT INTERACTIONS

**Progressive Solutions to Improve Corrosion Resistance for Nuclear Waste Storage — Corrosion and Aspects of Environmentally Safe Processing of Nuclear Waste Storage Materials**

**Sponsored by:** TMS Corrosion and Environmental Effects Committee, ACerS Glass & Optical Materials Division

**Program Organizers:** Madeleine Jordache, Stevens Institute of Technology; Gary Pickrell, Virginia Tech

Wednesday AM | October 20, 2021

A221 | Greater Columbus Convention Center

**Session Chairs:** Madeleine Jordache, Stevens Institute of Technology; Gary Pickrell, Virginia Tech

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10:20 AM Introductory Comments

10:25 AM

**Using Stress Modelling to Understand Effects of Pit Morphology on Stress Corrosion Cracking Initiation in Austenitic Stainless Steels:** *Alana Parey*<sup>1</sup>; <sup>1</sup>The Ohio State University

10:45 AM

**A Geopolymer for Hanford Secondary Waste:** *Sepideh Akhbari*<sup>1</sup>; Weiliang Gong<sup>1</sup>; Werner Lutze<sup>1</sup>; Ian Pegg<sup>1</sup>; <sup>1</sup>Catholic University of America -Vitreous State Lab

11:05 AM Invited

**Understanding Corrosion of Nuclear Waste Glasses through Molecular Dynamics Simulations and Quantitative Structural Property Relationship Analysis:** *Jincheng Du*<sup>1</sup>; <sup>1</sup>University of North Texas

11:35 AM Invited

**Predicting Zeolites' Stability during the Corrosion of Nuclear Waste Immobilization Glasses:** *Mathieu Bauchy*<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

## CERAMIC AND GLASS MATERIALS

### Solid-state Optical Materials and Luminescence Properties — Session I

**Sponsored by:** ACerS Basic Science Division, ACerS Engineering Ceramics Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Yiquan Wu, Alfred University; Jas Sanghera, Naval Research Laboratory; Akio Ikesue, World-Lab. Co., Ltd; Rong-Jun Xie, Xiamen University; Mathieu Allix, University of Orleans; Kiyoshi Shimamura, National Institute for Materials Science; Liangbi Su, Shanghai Institute of Ceramics; Dariusz Hreniak, Institute of Low Temperature and Structure Research

**Wednesday AM | October 20, 2021**  
**B232 | Greater Columbus Convention Center**

**Session Chairs:** Yiquan Wu, Alfred University; Jas Sanghera, Naval Research Laboratory

#### 8:00 AM Invited

**Non Rule-of-mixtures Thermal Expansion in Core-shell Based Nanocrystalline Composite Ceramics:** *James Wollmershauser*<sup>1</sup>; Kevin Anderson<sup>2</sup>; Benjamin Greenberg<sup>2</sup>; Heonjune Ryou<sup>1</sup>; Edward Gorzkowski<sup>1</sup>; Boris Feigelson<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory; <sup>2</sup>National Research Council Postdoctoral Research Fellow sited at U.S. Naval Research Laboratory

#### 8:20 AM

**Processing of Rare Earth Doped Ga<sub>2</sub>O<sub>3</sub> Transparent Ceramics:** *Jiao Li*<sup>1</sup>; Yiquan Wu<sup>1</sup>; <sup>1</sup>Alfred University

#### 8:40 AM Invited

**Additive Manufacturing of Tailored Laser Gain Media:** *Steve Payne*<sup>1</sup>; Zachary Seeley<sup>1</sup>; Nerine Cherepy<sup>1</sup>; Thomas Rudzik<sup>1</sup>; Tyler Wineger<sup>1</sup>; Ian Phillips<sup>1</sup>; Alex Drobshoff<sup>1</sup>; Tim Yee<sup>1</sup>; <sup>1</sup>Lawrence Livermore Lab

#### 9:00 AM

**Optical Basicity of Oxynitrides:** *Doris Möncke*<sup>1</sup>; Sharafat Ali<sup>2</sup>; Bo Jonson<sup>2</sup>; Efstratios Kamitsos<sup>3</sup>; <sup>1</sup>Alfred University; <sup>2</sup>Linnaeus University; <sup>3</sup>National Hellenic Research Foundation

#### 9:20 AM

**Highly Transparent MgGa<sub>2</sub>O<sub>4</sub> and Ni Doped MgGa<sub>2</sub>O<sub>4</sub> Semiconducting Ceramics:** *Guangran Zhang*<sup>1</sup>; Yiquan Wu<sup>1</sup>; <sup>1</sup>Alfred University

#### 9:40 AM Invited

**A Review of Sharp Indentation to Probe Contact Damage in Glass:** Brian Davis<sup>1</sup>; *Ivar Reimanis*<sup>1</sup>; Amanda Bellafatto<sup>1</sup>; Amber Tremper<sup>2</sup>; Scott Glaesemann<sup>2</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Corning Incorporated

## SPECIAL TOPICS

### ACerS Robert B. Sosman Award Symposium: Bridging the Gap between Atomistic and Continuum Approaches to Interface Science — Sosman Presentation

**Sponsored by:** ACerS Basic Science Division

**Program Organizer:** John Blendell, Purdue University

**Wednesday PM | October 20, 2021**  
**B130 | Greater Columbus Convention Center**

**Session Chair:** John Blendell, Purdue University

#### 1:00 PM Invited

**Combining Atomistic and Continuum Approaches Towards Understanding Interfaces:** *Wayne Kaplan*<sup>1</sup>; <sup>1</sup>Technion - Israel Institute of Technology

## SPECIAL TOPICS

### ACerS Robert B. Sosman Award Symposium: Bridging the Gap between Atomistic and Continuum Approaches to Interface Science — Sosmann II

**Sponsored by:** ACerS Basic Science Division

**Program Organizer:** John Blendell, Purdue University

**Wednesday PM | October 20, 2021**  
**B130 | Greater Columbus Convention Center**

**Session Chair:** Carol Handwerker, Purdue University

#### 2:00 PM Invited

**Grain Boundaries in the Wild:** *Gregory Rohrer*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

#### 2:30 PM Invited

**Stress-Induced Interface Instability in Battery Electrode Materials:** *Ming Tang*<sup>1</sup>; <sup>1</sup>Rice University

#### 3:00 PM Invited

**Tracing Impurities at Surfaces and Interfaces of Renewable Energy Materials:** *Christina Scheu*<sup>1</sup>; Joohyun Lim<sup>1</sup>; Se-Ho Kim<sup>1</sup>; Raquel Aymerich Armengol<sup>1</sup>; Rajib Sahu<sup>1</sup>; Olga Kasian<sup>1</sup>; Leigh T. Stephenson<sup>1</sup>; Baptiste Gault<sup>1</sup>; <sup>1</sup>Max-Planck-Institut fuer Eisenforschung GmbH

#### 3:30 PM Break

#### 3:50 PM Invited

**Surface Segregation in Multicomponent High Entropy Alloys: A Comparison between Atomistic Simulations and a Simple Analytical Model:** *Paul Wynblatt*<sup>1</sup>; Dominique Chatain<sup>2</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Aix-Marseille Univ, CNRS, CINAM

#### 4:20 PM Invited

**Disconnections, Faceting, Solutes and Their Impact on Grain Boundary Migration in Ceramics:** *Rheinheimer Wolfgang*<sup>1</sup>; Hadas Sternlicht<sup>2</sup>; <sup>1</sup>Forschungszentrum Jülich; <sup>2</sup>Brown University

# Technical Program

4:50 PM Invited

**Mechanistic Insights into the Effect of Heating Rate on Sintering and Sintering Stress Evolution:** *Shen Dillon<sup>1</sup>*; <sup>1</sup>University of Illinois

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## ADDITIVE MANUFACTURING

**Additive Manufacturing of High and Ultra-High Temperature Ceramics and Composites: Processing, Characterization and Testing — Extrusion-based Additive Manufacturing Methods**

*Sponsored by:* ACerS Engineering Ceramics Division

**Program Organizers:** Corson Cramer, Oak Ridge National Laboratory; Greg Hilmas, Missouri University of Science and Technology; Lisa Rueschhoff, Air Force Research Laboratory

Wednesday PM | October 20, 2021

A111 | Greater Columbus Convention Center

**Session Chair:** Greg Hilmas, Missouri University of Science and Technology

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2:00 PM

**Additive Manufacturing Of ZrB<sub>2</sub>-SiC Heat Exchanger Geometries by Ceramic on Demand Extrusion:** *Nicholas Timme<sup>1</sup>*; Marharyta Lakusta<sup>1</sup>; Jeremy Watts<sup>1</sup>; Gregory Hilmas<sup>1</sup>; William Fahrenholtz<sup>1</sup>; Ming Leu<sup>1</sup>; David Lipke<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

2:20 PM

**Ceramic On-demand Extrusion (CODE) of Functionally Graded ZrB<sub>2</sub>-Mo:** *Austin Martin<sup>1</sup>*; Sachin Choudhary<sup>1</sup>; Jeremy Watts<sup>1</sup>; Gregory Hilmas<sup>1</sup>; Ming Leu<sup>1</sup>; Tieshu Huang<sup>2</sup>; <sup>1</sup>Missouri University of Science and Technology; <sup>2</sup>NNSA's Kansas City National Security Campus

2:40 PM

**Additive Manufacturing of Aqueous Based Silicon Nitride Suspensions via Direct Writing:** *William Costakis<sup>1</sup>*; Connor Wyckoff<sup>1</sup>; Lisa Rueschhoff<sup>1</sup>; <sup>1</sup>Air Force Research Labs

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## ADDITIVE MANUFACTURING

**Additive Manufacturing of Metals: Equipment, Instrumentation and In-Situ Process Monitoring — Novel Instrumentation**

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Joy Gockel, Colorado School of Mines; Sneha Prabha Narra, Carnegie Mellon University

Wednesday PM | October 20, 2021

A121 | Greater Columbus Convention Center

**Session Chair:** Joy Gockel, Colorado School of Mines

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3:00 PM Invited

**Ultrasonics for Monitoring Melt Pool Dynamics and Solidification:** *Christopher Kube<sup>1</sup>*; Jared Gillespie<sup>1</sup>; Tao Sun<sup>2</sup>; Cang Zhao<sup>3</sup>; Niranjana Parab<sup>4</sup>; Anthony Rollett<sup>5</sup>; <sup>1</sup>The Pennsylvania State University; <sup>2</sup>University of Virginia; <sup>3</sup>Tsinghua University; <sup>4</sup>Intel Corporation; <sup>5</sup>Carnegie Mellon University

3:40 PM

**Functionally Graded Material Development by Leveraging Ultrasonic Grain Refinement in Additive Manufactured Nickel 718:** *Nathaniel McNees<sup>1</sup>*; Satish Rajaram<sup>2</sup>; Mark Warchol<sup>2</sup>; Brian Wisner<sup>1</sup>; <sup>1</sup>Ohio University; <sup>2</sup>Texas Research Institute-Austin

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## ADDITIVE MANUFACTURING

**Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Additive Manufacturing: Miscellaneous**

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

Wednesday PM | October 20, 2021

A120 | Greater Columbus Convention Center

**Session Chair:** Roman Maev, University of Windsor

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2:00 PM

**Additive Manufacturing of Metallic Materials: Mechanical Properties:** *Prashanth Konda Gokuldoss<sup>1</sup>*; <sup>1</sup>Tallinn University of Technology

2:20 PM

**Advancements in High Pressure Heat Treatment for AM Parts:** *Chad Beamer<sup>1</sup>*; <sup>1</sup>Quintus Technologies

2:40 PM

**Avoiding Deleterious Phase Formation in Abrupt Interface Bonding of Multi-material Structures:** *Nicholas Jones<sup>1</sup>*; Jack Beuth<sup>1</sup>; Maarten de Boer<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

3:00 PM

**Controlling High Temperature Mechanical Performance of Superalloys Fabricated via Laser Powder Bed Fusion through Processing Parameter Variation:** *Nicholas Lamprinakos<sup>1</sup>*; Joseph Pauza<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

3:20 PM

**Effects of Extrusion-based Additive Manufacturing on Thermoelectric Transport in Nickel and Bismuth:** *Victoria Stotzer<sup>1</sup>*; Christian Apel<sup>1</sup>; Sarah Watzman<sup>1</sup>; Ashley Paz y Puente<sup>1</sup>; <sup>1</sup>University of Cincinnati

3:40 PM Break

4:00 PM

**Location-specific Fatigue Life Predictions in AM Parts Using Physics-based Models within an ICME Framework:** *Manisha Banker<sup>1</sup>*; Ayman Salem<sup>1</sup>; Daniel Satko<sup>1</sup>; Jan Kasprzak<sup>2</sup>; Nam Phan<sup>2</sup>; <sup>1</sup>MRL Materials Resources LLC; <sup>2</sup>Naval Air Systems Command

4:20 PM

**Low Pressure Cold Spray Additive Manufacturing of Molds and Dies:** *Roman Maev<sup>1</sup>*; Volf Leshchynsky<sup>1</sup>; Ahmed Elseddawy<sup>1</sup>; Emil Strumban<sup>1</sup>; John Wladarski<sup>1</sup>; <sup>1</sup>IDIR

4:40 PM

**Microstructural and Electrochemical Properties of Additively Manufactured Alloys:** *Ali Raza<sup>1</sup>*; Sohaib Khan<sup>2</sup>; Waseem Haider<sup>1</sup>; <sup>1</sup>Central Michigan University; <sup>2</sup>Islamic University of Madinah

## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — Fe-based Alloys

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

**Wednesday PM | October 20, 2021**  
**A115 | Greater Columbus Convention Center**

**Session Chair:** Rangasayee Kannan, Oak Ridge National Laboratory

#### 2:00 PM

**Binder Jet Printing of Austenitic 316L Stainless Steel: Processing, Densification, Microstructure, and Mechanical Properties:** *M Jamalkhani Khameneh<sup>1</sup>; Amir Mostafaei<sup>2</sup>; <sup>1</sup>Illinois Institute of Technology*

#### 2:20 PM

**Deformation Mechanisms in 316L Stainless Steel Fabricated by Additive and Additive + Subtractive (Hybrid) Manufacturing:** *Rangasayee Kannan<sup>1</sup>; Peeyush Nandwana<sup>1</sup>; Thomas Feldhausen<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

#### 2:40 PM

**Influence of the Cellular Subgrain Feature in Additively Manufactured 316L Stainless Steel on Mechanical Properties:** *Janith Wanniarachchi<sup>1</sup>; John Michopoulos<sup>2</sup>; Ajit Achuthan<sup>1</sup>; <sup>1</sup>Clarkson University; <sup>2</sup>Naval Research Laboratory*

#### 3:00 PM

**Microstructural Evolution in Maraging Steels: From Powder to Additive Manufacturing:** *Seyedamirreza Shamsdin<sup>1</sup>; Mohsen Mohammadi<sup>1</sup>; <sup>1</sup>UNB*

#### 3:20 PM Break

#### 3:40 PM

**Mechanical Properties and Metallurgical Characteristics of H13 Tool Steel Additively Manufactured in Low Vacuum and Heated Condition:** *Shinji Matsushita<sup>1</sup>; Hirotsugu Kawanaka<sup>1</sup>; Hyakka Nakada<sup>1</sup>; Steven Osma<sup>1</sup>; Yusuke Yasuda<sup>1</sup>; Seung Hwan Park<sup>1</sup>; <sup>1</sup>Hitachi Ltd.*

#### 4:00 PM

**Nano and Macro Mechanical Properties of Additively and Traditionally Manufactured 17-4 PH Stainless Steel:** *Hisham Abusalma<sup>1</sup>; Mohammad Sepahi<sup>1</sup>; Sandeep Khadka<sup>1</sup>; Dana Ingalsbe<sup>1</sup>; Natalia Esparragoza<sup>1</sup>; Matthew Rosser<sup>1</sup>; Xiaoqing Wang<sup>1</sup>; *Hamid Eisazadeh<sup>1</sup>; <sup>1</sup>Old Dominion University**

#### 4:20 PM

**Use of Water Atomized Powder with Non-spherical Morphology in a Laser Powder Bed Fusion Additive Manufacturing Process:** *Mahya Shahabi<sup>1</sup>; Tianyu Zhu<sup>1</sup>; Jagannath Jayachandran<sup>1</sup>; Sneha Prabha Narra<sup>2</sup>; <sup>1</sup>Worcester Polytechnic Institute; <sup>2</sup>Carnegie Mellon University*

## ADDITIVE MANUFACTURING

### Additive Manufacturing: Large-Scale Metal Additive Manufacturing — Microstructure, Property, and Performance: Characterization and Simulation

**Program Organizers:** Yousub Lee, Oak Ridge National Laboratory; Antonio Ramirez, Ohio State University; Yashwanth Bandari, Meltio Inc.; Duckbong Kim, Tennessee Technological University; Wei Zhang, Ohio State University

**Wednesday PM | October 20, 2021**  
**A114 | Greater Columbus Convention Center**

**Session Chairs:** Kaiwen Zhang, The Ohio State University; Antonio Ramirez, The Ohio State University

#### 2:00 PM

**Wire Arc Processing of Stainless Steels; Microstructure and Properties:** *Patxi Fernandez-Zelaia<sup>1</sup>; Quinn Campbell<sup>1</sup>; Chris Ledford<sup>1</sup>; Michael Kirka<sup>1</sup>; Andrzej Nycz<sup>1</sup>; Mark Noakes<sup>1</sup>; Lonnie Love<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

#### 2:30 PM

**Effect of Inhomogeneous Grain Size on the Deformation Characteristics of Bimetallic Additively Manufactured Structure (BAMS) of 316L Austenitic Stainless Steel and Inconel 625:** *Rumman Ahsan<sup>1</sup>; Xuesong Fan<sup>2</sup>; Jonathan Poplawsky<sup>3</sup>; Peter Liaw<sup>2</sup>; Duck Bong Kim<sup>1</sup>; <sup>1</sup>Tennessee Technological University; <sup>2</sup>University of Tennessee, Knoxville; <sup>3</sup>Oak Ridge National Laboratory*

#### 2:50 PM

**Microstructure Modification of GMAW-DED 316L Stainless Steel:** *Jacob Rindler<sup>1</sup>; Antonio Ramirez<sup>1</sup>; <sup>1</sup>Ohio State University*

#### 3:10 PM

**Towards Understanding Microstructure Evolution during Wire Arc Additive Manufacturing of Maraging 250 Thin-wall Parts:** *Yao Xu<sup>1</sup>; Brajendra Mishra<sup>1</sup>; Sneha Narra<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute*

#### 3:30 PM Break

#### 3:50 PM

**Wire + Arc Additive Manufacturing (WAAM) of Al0.1CoCrFeNi High-Entropy Alloy (HEA):** *Rumman Ahsan<sup>1</sup>; Xuesong Fan<sup>2</sup>; Jonathan Poplawsky<sup>3</sup>; Peter Liaw<sup>2</sup>; Duck Bong Kim<sup>1</sup>; <sup>1</sup>Tennessee Technological University; <sup>2</sup>University of Tennessee, Knoxville; <sup>3</sup>Oak Ridge National Laboratory*

#### 4:10 PM

**Process Development for Laser Hot Wire Additive Manufacturing of Ti-6Al-4V:** *Elizabeth Chang-Davidson<sup>1</sup>; Brandon Abranovic<sup>1</sup>; Jack Beuth<sup>1</sup>; <sup>1</sup>Carnegie Mellon University*

#### 4:30 PM

**A Machine Learning-based Geometric Compensation Method for Metal Additive Manufacturing:** *Wen Dong<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh*



# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Mechanisms and Mitigation of Aqueous Corrosion and High-temperature Oxidation — Corrosion Assessment of Additively Manufactured Parts II

**Program Organizers:** Amir Mostafaei, Illinois Institute of Technology; Yashar Behnamian, University of Alberta; Bryan Webler, Carnegie Mellon University

**Wednesday PM | October 20, 2021**  
**A112 | Greater Columbus Convention Center**

**Session Chair:** To Be Announced

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#### 2:00 PM

**Influence of Heat Treatment on Electrochemical Behavior of Additively Manufactured 7050 Aluminum Alloy:** *Rupesh Rajendran*<sup>1</sup>; Kevin Chasse<sup>2</sup>; Preet Singh<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>Northrop Grumman Mission Systems

#### 2:30 PM

**Electrochemical Behavior of Additively-manufactured Steels:** *M Jamalkhani Khameneh*<sup>1</sup>; Amir Mostafaei<sup>1</sup>; <sup>1</sup>Illinois Institute of Technology

#### 3:00 PM

**Corrosion Behavior of Additively Manufactured Parts Made Using Non-spherical Ti-6Al-4V Powder in 3.5 wt% NaCl Solution:** Sourabh Bagi<sup>1</sup>; Muktesh Paliwal<sup>2</sup>; Anthony Rollett<sup>3</sup>; *Amir Mostafaei*<sup>1</sup>; <sup>1</sup>Illinois Institute of Technology; <sup>2</sup>Kymera International - Reading Alloys; <sup>3</sup>Carnegie Mellon University

#### 3:30 PM Break

#### 3:50 PM

**Laser Shock Peening Effect on 5xxx Sensitization and Exfoliation of 5XXX series Aluminum Alloys:** Saba N. Esmaeely<sup>1</sup>; Allison Akman<sup>2</sup>; Gabriella Marino<sup>1</sup>; *Jenifer Locke*<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Naval Surface Warfare Center,

#### 4:20 PM

**Corrosion Behavior of Laser Powder Bed Fusion Processed Ti-6Al-4V in Different Electrolytes:** *Melody Delpazir*<sup>1</sup>; Muktesh Paliwal<sup>2</sup>; Marcella Vaicik<sup>1</sup>; Amir Mostafaei<sup>1</sup>; <sup>1</sup>Illinois Institute of Technology; <sup>2</sup>Kymera International - Reading Alloys

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Session IV

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**Wednesday PM | October 20, 2021**  
**A223 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

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#### 2:00 PM

**Passive Wireless Sensors for Real Time Temperature and Corrosion Monitoring of Coal Boiler Components Under Flexible Operation:** *Brian Jordan*<sup>1</sup>; Kavin Idhaiah<sup>1</sup>; Zachary Lynch<sup>1</sup>; Daryl Reynolds<sup>1</sup>; Edward Sabolsky<sup>1</sup>; <sup>1</sup>WVU

#### 2:20 PM

**Development of High Performance H<sub>2</sub> Permeation Barrier Coating with Good Thermal Cycling Resistance:** *Sumit Bhattacharya*<sup>1</sup>; Yinbin Miao<sup>1</sup>; Nicholas Stauff<sup>1</sup>; Taek Kim<sup>1</sup>; Abdellatif Yacout<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

#### 2:40 PM

**Influence of Alkaline Earth Metals on Structure Formation, Mechanical and Special Properties of Aircraft Casting from Magnesium Alloys:** Vadim Shalomeev<sup>1</sup>; Sergei Sheyko<sup>1</sup>; *Ievgeniia Chetvertak*<sup>1</sup>; <sup>1</sup>National University "Zaporizhka Politechnics"

#### 3:00 PM

**Microstructural Stability at Elevated Temperature of the Ni-based Electron Beam Welded Superalloys Dissimilar Joint:** Oskar Dziuba<sup>1</sup>; Grzegorz Cempura<sup>1</sup>; *Agnieszka Wusatowska-Sarnek*<sup>2</sup>; Adam Kruk<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology; <sup>2</sup>Pratt & Whitney

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Session V

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**Wednesday PM | October 20, 2021**  
**A224 | Greater Columbus Convention Center**

**Session Chairs:** Gary Pickrell, Professor, Virginia Tech; Navin Manjooran, Chairman, Solve

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#### 2:00 PM

**Corrosion Behaviors of Alloys in High Temperature Supercritical CO<sub>2</sub> with Impurity:** Yimin Zeng<sup>1</sup>; *Kaiyang Li*<sup>1</sup>; <sup>1</sup>NRCan, Canada

**2:20 PM**

**Assessment of Conductive Sites on Carbon Fiber Reinforced Polymer Composite Using Different Electrochemical Experimental Methods:** Priyanka Adapala<sup>1</sup>; <sup>1</sup>The Ohio State University

**2:40 PM**

**The Importance of Quality Control, Characterization and Testing in Manufacturing and Production:** Jeanette Vass<sup>1</sup>; <sup>1</sup>Auto and Materials

**3:00 PM**

**Scandium-containing Filler Material for Welding Aircraft Castings Made of High-temperature Magnesium-based Alloy:** Vadim Shalomeev<sup>1</sup>; Sergei Sheyko<sup>2</sup>; Ievgeniia Chetvertak<sup>1</sup>; <sup>1</sup>National University "Zaporizhska Politechnics"; <sup>2</sup>Zaporizhzhia National University

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**CERAMIC AND GLASS MATERIALS**

**Ceramics and Glasses Modeling by Simulations and Machine Learning — Session II**

**Sponsored by:** ACerS Glass & Optical Materials Division

**Program Organizers:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**Wednesday PM | October 20, 2021**  
**B231 | Greater Columbus Convention Center**

**Session Chairs:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**2:00 PM**

**Ceramics from Polymers -- Results of Ab Initio Molecular Dynamic Simulations:** Peter Kroll<sup>1</sup>; <sup>1</sup>University of Texas at Arlington

**2:20 PM**

**Fusing Experimental and Simulation Datasets in Machine Learning for Predicting Glass Properties:** Mathieu Bauchy<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

**2:40 PM**

**Bayesian Optimization of Silicon Nitride Empirical Potentials:** Tobias Kroll<sup>1</sup>; Peter Kroll<sup>1</sup>; <sup>1</sup>University of Texas at Arlington

**3:00 PM**

**Development of a Reactive Force Field (ReaxFF) for Simulation of Polymer-derived Ceramics:** Shariq Haseen<sup>1</sup>; Peter Kroll<sup>1</sup>; <sup>1</sup>University of Texas at Arlington

**3:20 PM Panel Discussion:** Challenges and Opportunities in Machine Learning for Materials

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**MATERIALS-ENVIRONMENT INTERACTIONS**

**Computation Assisted Materials Development for Improved Corrosion Resistance — B: High Temperature Corrosion**

**Program Organizers:** Rishi Pillai, Oak Ridge National Laboratory; Laurence Marks, Northwestern University

**Wednesday PM | October 20, 2021**  
**A222 | Greater Columbus Convention Center**

**Session Chair:** David Shifler, Office of Naval Research

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**2:00 PM Introductory Comments**

**2:05 PM**

**Hydrothermal Corrosion of Silicon Carbide:** Jianqi Xi<sup>1</sup>; Dane Morgan<sup>1</sup>; Izabela Szlufarska<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**2:25 PM**

**Solubility Based Prediction of Corrosion in Molten Chloride Salts:** Cory Parker<sup>1</sup>; Rishi Pillai<sup>1</sup>; Dino Sulejmanovic<sup>1</sup>; Bruce Pint<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**2:45 PM**

**Understanding and Reducing Bias in Machine Learning to Enhance Its Predictive and Extrapolative Capabilities: Application to the Oxidation Kinetics and Spallation Behavior of High-temperature NiCr-based Alloys:** Marie Romedenne<sup>1</sup>; Rishi Pillai<sup>1</sup>; Jian Peng<sup>1</sup>; Bruce Pint<sup>1</sup>; Allen Haynes<sup>1</sup>; Govindarajan Muralidharan<sup>1</sup>; Dongwon Shin<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

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**NANOMATERIALS**

**Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — Nanoparticles & Nanocomposites II**

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**Wednesday PM | October 20, 2021**  
**B240/241 | Greater Columbus Convention Center**

**Session Chairs:** Kathy Lu, Virginia Tech; Edward Gorzkowski, Naval Research Laboratory

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**2:00 PM**

**Bulk Nanostructured Ceramics Research at the US Naval Research Lab:** Edward Gorzkowski<sup>1</sup>; James Wollmershauser<sup>1</sup>; Eric Patterson<sup>1</sup>; Heonjune Ryou<sup>1</sup>; Kevin Anderson<sup>1</sup>; Boris Feigelson<sup>1</sup>; <sup>1</sup>Naval Research Laboratory

# Technical Program

**2:20 PM Invited**

**Polymer Derived Ceramics and Composites- From Nanoscale to Bulk Properties:** *Lisa Rueschhoff<sup>1</sup>; Zlatomir Apostolov<sup>1</sup>; Matthew Dickerson<sup>1</sup>; Michael Cinibulk<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory*

**2:50 PM Invited**

**Polymer-Derived Ceramic Nanocomposites for Applications at High Temperatures and in Harsh Environments:** *Emanuel Ionescu<sup>1</sup>; <sup>1</sup>TU Darmstadt*

**3:20 PM**

**Sintering, Structure, and Properties of  $Y_2O_3$ - $ZrO_2$ - $Al_2O_3$  Core-Shell Nanocomposite Ceramics:** *Kevin Anderson<sup>1</sup>; Benjamin Greenberg<sup>1</sup>; Mason Wolak<sup>1</sup>; James Wollmershauser<sup>1</sup>; Boris Feigelson<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory*

## FUNDAMENTALS AND CHARACTERIZATION

### Emergent Materials under Extremes and Decisive $\langle I \rangle$ In Situ Characterizations — Materials Characterization at Extreme Conditions

**Sponsored by:** ACerS Basic Science Division

**Program Organizers:** Hongwu Xu, Los Alamos National Laboratory; Xiaofeng Guo, Washington State University; Xujie Lu, Center for High Pressure Science & Technology Advanced Research; Hua Zhou, Argonne National Laboratory; Judith Driscoll, University of Cambridge

**Wednesday PM | October 20, 2021**

**B244/245 | Greater Columbus Convention Center**

**Session Chairs:** Hongwu Xu, Los Alamos National Laboratory; Xiaofeng Guo, Washington State University; Hua Zhou, Argonne National Laboratory

**2:00 PM Invited**

**In-Situ Synchrotron X-ray Absorption Spectroscopic Investigations of Actinide Speciation under Hydrothermal Conditions:** *Robert Mayanovic<sup>1</sup>; Jason Baker<sup>2</sup>; Diwash Dhakal<sup>1</sup>; Nadib Akram<sup>1</sup>; Xiaofeng Guo<sup>3</sup>; Hakim Boukhalfa<sup>2</sup>; Cheng-Jun Sun<sup>4</sup>; Hongwu Xu<sup>2</sup>; <sup>1</sup>Missouri State University; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>Washington State University; <sup>4</sup>Argonne National Laboratory*

**2:20 PM**

**In-situ Two-dimensional X-ray Diffraction (XRD2) Studies On High-temperature Phase Transformations of 2D Titanium Carbide ( $Ti_3C_2Tx$ ) MXene:** *Brian Wyatt<sup>1</sup>; Srinivasa Kartik Neman<sup>1</sup>; Bowen Zhang<sup>1</sup>; Babak Anasori<sup>1</sup>; <sup>1</sup>Integrated Nanosystems Development Institute (INDI), IUPUI*

**2:40 PM Invited**

**Proton Irradiation Effects in Additively Manufactured 316L Stainless Steels:** *Cheng Sun<sup>1</sup>; Michael McMurtrey<sup>1</sup>; <sup>1</sup>Idaho National Laboratory*

**3:00 PM**

**Temperature Measurements in Radiation Environments Using Piezoelectric Surface Acoustic Wave Resonators:** *Maha Yazbeck<sup>1</sup>; Ryan Chesser<sup>1</sup>; Yuzhou Wang<sup>2</sup>; Marat Khafizov<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Idaho National Lab*

## ENERGY

### Energy Materials for Sustainable Development — Capacitative, Chemical and Thermal Storage and Conversion

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

**Wednesday PM | October 20, 2021**

**A216 | Greater Columbus Convention Center**

**Session Chairs:** Kevin Huang, University of South Carolina; Kyle Brinkman, Clemson University

**2:00 PM Invited**

**Thermomagnetic Transport in 2D Layered Materials:** *Mona Zebarjadi<sup>1</sup>; Md. Sabbir Akhanda<sup>1</sup>; Emad Rezaei<sup>1</sup>; <sup>1</sup>University of Virginia*

**2:30 PM Invited**

**Synthesis of New Antimonides for Thermoelectric Applications:** *Julia Zaikina<sup>1</sup>; <sup>1</sup>Iowa State University*

**2:50 PM**

**Enhancement of Thermoelectric Properties of Bismuth Sulfide by Halide Substitution:** *Farheen Anjum<sup>1</sup>; <sup>1</sup>IIT Kanpur*

## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Processing and Properties III

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Wednesday PM | October 20, 2021**

**B132 | Greater Columbus Convention Center**

**Session Chair:** Fei Wang, University of Nebraska Lincoln

**2:00 PM**

**Behavior of a High-entropy Alloy in Molten Salt Environments under Biaxial Stresses:** *Wylie Simpson<sup>1</sup>; James Earthman<sup>1</sup>; Xinyi Wang<sup>1</sup>; <sup>1</sup>University of California Irvine*

**2:20 PM**

**Control of Local Distortions in High-entropy Oxides:** *Keivan Esfarjani<sup>1</sup>; Jonathan Kaufman<sup>1</sup>; <sup>1</sup>University of Virginia*

**2:40 PM**

**Microstructure and Phase Stability of High Entropy (RE)PO<sub>4</sub> Monazite-structured Ceramics:** *Nadja Motley<sup>1</sup>; Adriana Mejia<sup>1</sup>; Yingie Yang<sup>1</sup>; Daniel Mumm<sup>1</sup>; Martha Mecartney<sup>1</sup>; <sup>1</sup>University of California, Irvine*

**3:00 PM**

**Surface Enhancement of Multi-principal Element Alloys by Gas Nitriding:** *Yu-Hsuan Lin<sup>1</sup>; David Poerschke<sup>1</sup>; <sup>1</sup>University of Minnesota*

**3:20 PM**

**Structural and Mechanical Properties of High Entropy Metal-nitride:** *Saro San<sup>1</sup>; Wai-Yim Ching<sup>2</sup>; <sup>1</sup>University of Missouri; <sup>2</sup>University of Missouri Kansas City*

**3:40 PM Break**

**4:00 PM**

**Multi-component High Entropy Ultra-high Temperature Carbides: Solid-solution to High-entropy Phase Formation:** *Ambreen Nisar<sup>1</sup>; Tyler Dolmetsch<sup>1</sup>; Tanaji Paul<sup>1</sup>; Cheng Zhang<sup>1</sup>; Benjamin Boesl<sup>1</sup>; Arvind Agarwal<sup>1</sup>; <sup>1</sup>Florida International University*

**4:20 PM**

**The Dynamic and Sensing Performance of 3D Printed Functionally Graded Elastomeric Lattice Structures:** *Charles Dwyer<sup>1</sup>; Joao Garretto<sup>1</sup>; Ronald Yarwood<sup>1</sup>; Jae-Won Choi<sup>2</sup>; Eric MacDonald<sup>3</sup>; Pedro Cortes<sup>1</sup>; Gina Morrison<sup>1</sup>; <sup>1</sup>Youngstown State University; <sup>2</sup>University of Akron; <sup>3</sup>The University of Texas at El Paso*

**4:40 PM**

**Temperature Dependent Mechanical Behavior of the Au-Zn-Al Ternary System:** *Taylor Jacobs<sup>1</sup>; Seth Imhoff<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory*

**5:00 PM**

**The Research Thermoplastic Deformation Modes of Dual-phase Special Alloys for Obtaining Rational Intermetallic Structure:** *Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Irina Kruglyak<sup>1</sup>; Yuriy Belokon<sup>2</sup>; <sup>1</sup>Dneprovsky State Technical University; <sup>2</sup>Zaporizhzhya National University*

**FUNDAMENTALS AND CHARACTERIZATION**

**High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — Theory and Modeling II**

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

**Wednesday PM | October 20, 2021**

**B131 | Greater Columbus Convention Center**

**Session Chairs:** Mike Widom, Carnegie Mellon University; Stefano Curtarolo, Duke University

**2:00 PM Invited**

**To Mix, or not to Mix: Progresses in Entropy Descriptors:** *Stefano Curtarolo<sup>1</sup>; <sup>1</sup>Duke University*

**2:30 PM Invited**

**Development of Interatomic Potentials for Highly Concentrated/Entropy-stabilized Systems:** *Ridwan Sakidja<sup>1</sup>; Andrew Duff<sup>2</sup>; Bikash Timalsina<sup>1</sup>; Tyler McGilvry-James<sup>1</sup>; <sup>1</sup>Missouri State University; <sup>2</sup>Daresbury Laboratory*

**2:50 PM Invited**

**First-principles Predictions of Chemical Short-range Order in High Entropy Alloys:** *Michael Widom<sup>1</sup>; <sup>1</sup>Carnegie Mellon University*

**3:20 PM Break**

**3:40 PM Invited**

**Temperature-dependent Configurational Entropy Calculations for Refractory High-entropy Alloys:** *Chiraag Nataraj<sup>1</sup>; Axel van de Walle<sup>1</sup>; Amit Samanta<sup>2</sup>; <sup>1</sup>Brown University; <sup>2</sup>Lawrence Livermore National Lab*

**4:00 PM Invited**

**Phase-field Modelling of Transformation Pathways and Microstructural Evolution in MPEAs (Multi Principal Element Alloys):** *Kamal Nath Kadirvel<sup>1</sup>; Jacob Jensen<sup>1</sup>; Zachary Kloenne<sup>1</sup>; Rajarshi Banerjee<sup>2</sup>; Hamish Fraser<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>University of North Texas*

**4:20 PM**

**Atomistic Simulations of the Structure and Mechanical Properties of Grain Boundaries in High Entropy Alloys:** *Fadi Abdeljawad<sup>1</sup>; <sup>1</sup>Clemson University*

**CERAMIC AND GLASS MATERIALS**

**Journal of the American Ceramic Society Awards Symposium — Journal of the American Ceramic Society Awards Symposium II**

**Sponsored by:** ACerS

**Program Organizer:** William Fahrenholtz, Missouri University of Science and Technology

**Wednesday PM | October 20, 2021**

**B233 | Greater Columbus Convention Center**

**Session Chairs:** William Fahrenholtz, Missouri University of Science and Technology; Jonathon Foreman, American Ceramic Society

**2:00 PM Invited**

**In-Situ Resistance Degradation & Switching of Bulk YSZ & STO Single Crystals:** *Ana Alvarez<sup>1</sup>; I-Wei Chen<sup>1</sup>; <sup>1</sup>University of Pennsylvania*

**2:30 PM Invited**

**Glassy Ga-Te Binaries: Structure and Properties for Phase-change Memory Applications:** *Andrey Tverjanovich<sup>1</sup>; Maria Bokova<sup>2</sup>; Chris Benmore<sup>3</sup>; Daniele Fontanari Fontanari<sup>2</sup>; Anton Sokolov<sup>2</sup>; Mohammad Kassem<sup>2</sup>; Maxim Khomenko<sup>4</sup>; Eugene Bychkov<sup>5</sup>; <sup>1</sup>Institute of Chemistry, Saint Petersburg State University; <sup>2</sup>Université du Littoral Côte d'Opale; <sup>3</sup>Advanced Photon Source, Argonne National Laboratory; <sup>4</sup>ILIT RAS-Branch of the FSRC "Crystallography and Photonics" RAS; <sup>5</sup>Université du Littoral Côte d'Opale; ILIT RAS-Branch of the FSRC "Crystallography and Photonics" RAS*

**3:00 PM Break**

**3:30 PM Invited**

**Domain Walls in Ferroelectrics:** *Sukriti Mantri<sup>1</sup>; John Daniels<sup>1</sup>; <sup>1</sup>University of New South Wales*



# Technical Program

4:00 PM Invited

**Relaxor Characteristics and Electromechanical Response under High Field for Sodium Bismuth Titanate-based Ceramics:** *Shuaishuai Bian<sup>1</sup>; Zhenxing Yue<sup>1</sup>; <sup>1</sup>Tsinghua University*

4:30 PM Concluding Comments

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## ARTIFICIAL INTELLIGENCE

### Materials Informatics for Images and Multi-dimensional Datasets — Session II

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Amanda Krause, University of Florida; Alp Sehirlioglu, Case Western Reserve University; Daniel Ruscitto, General Electric

Wednesday PM | October 20, 2021  
A124 | Greater Columbus Convention Center

**Session Chairs:** Amanda Krause, University of Florida; Kimberly Gliebe, Case Western Reserve University

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2:00 PM

**Characterization of Additively Manufactured ZrB<sub>2</sub>-SiC Ultra High Temperature Ceramics via X-ray Microtomography:** *Pratish Rao<sup>1</sup>; Jonghyun Park<sup>1</sup>; Jeremy Watts<sup>1</sup>; William Fahrenholtz<sup>1</sup>; Gregory Hilmas<sup>1</sup>; David Lipke<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology*

2:20 PM

**Computational or Experimental? Interpreting X-ray Absorption and Diffraction Contrast for Massive Non-destructive 3D Grain Mapping of Metals in Laboratory CT:** *Andy Holwell<sup>1</sup>; Hrishikesh Bale<sup>2</sup>; <sup>1</sup>Carl Zeiss Microscopy Ltd.; <sup>2</sup>Carl Zeiss Microscopy Inc.*

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## CERAMIC AND GLASS MATERIALS

### Preceramic Polymers; Synthesis, Processing, Modeling, and Derived Ceramics — Preceramic Polymers and Polymer Derived Ceramics II

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Matthew Dickerson, Air Force Research Laboratory; Gurpreet Singh, Kansas State University; Paolo Colombo, University of Padova; Günter Motz, Universität Bayreuth

Wednesday PM | October 20, 2021  
B230 | Greater Columbus Convention Center

**Session Chair:** Gurpreet Singh, Kansas State University

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2:00 PM

**Effect of Pendant Groups on the Mass Yield, Density and Process Modeling of Polycarbosilanes during Pyrolysis:** *Thomas Key<sup>1</sup>; Garth Wilks<sup>2</sup>; Michael Cinibulk<sup>2</sup>; <sup>1</sup>UES Inc; <sup>2</sup>Materials & Manufacturing Directorate, Air Force Research Laboratory, RXCC*

2:20 PM Invited

**Atomistic Simulations of Polymer Pyrolysis:** *Peter Kroll<sup>1</sup>; <sup>1</sup>University of Texas at Arlington*

2:50 PM

**Organics Matter: Common Features in Energetics of Polymer Derived Ceramics, Metal Organic Frameworks, and other Hybrid Materials:** *Alexandra Navrotsky<sup>1</sup>; <sup>1</sup>Arizona State University*

3:10 PM

**Thermal and Rheological Properties of Preceramic Polymer Grafted Nanoparticles:** *Kara Martin<sup>1</sup>; Ravichandran Kollarigowda<sup>2</sup>; Caitlyn Clarkson<sup>3</sup>; Christina Thompson<sup>4</sup>; Subramanian Ramakrishnan<sup>2</sup>; Matthew Dickerson<sup>5</sup>; <sup>1</sup>UES, Inc; <sup>2</sup>FAMU-FSU College of Engineering; <sup>3</sup>NRC Research Associateship Program; <sup>4</sup>Southwest Ohio Council for Higher Education (SOCHE) Program; <sup>5</sup>Air Force Research Lab*

3:30 PM Break

3:50 PM Invited

**Molecules, Polymers, and Rings: Preceramic Compounds for AsB Formation:** *Brandon Ackley<sup>1</sup>; Rory Waterman<sup>2</sup>; <sup>1</sup>ARCTOS Technology Solutions; <sup>2</sup>University of Vermont*

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## FUNDAMENTALS AND CHARACTERIZATION

### Processing—Microstructure—Property Relationships of Titanium and Titanium Alloys — Session II

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Yufeng Zheng, University of Nevada-Reno; Rongpei Shi, Lawrence Livermore National Laboratory; Michael Gram, Titanium Metals Corporation

Wednesday PM | October 20, 2021  
B246 | Greater Columbus Convention Center

**Session Chairs:** Michael Gram, Titanium Metals Corporation; Yufeng Zheng, University of Nevada Reno

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2:00 PM

**Computational Polarized-Light Microscopy for Microtextured Regions Characterization in Titanium Alloys:** *Matthew Dahar<sup>1</sup>; Sesh Tamirisakandala<sup>1</sup>; Dan Satko<sup>2</sup>; Ayman Salem<sup>2</sup>; <sup>1</sup>Howmet Aerospace; <sup>2</sup>Materials Resources, LLC*

2:20 PM

**Computational Polarized Light Microscopy for Orientation-based Quality Control:** *Daniel Satko<sup>1</sup>; Thomas Carmody<sup>1</sup>; Chasen Ranger<sup>1</sup>; Sesh Tamirisakandala<sup>2</sup>; Matthew Dahar<sup>2</sup>; Ayman Salem<sup>1</sup>; <sup>1</sup>MRL Materials Resources LLC; <sup>2</sup>Howmet Aerospace*

2:40 PM

**Strain Energy Density Fatigue Assessment of Ti-6Al-4V for Plain and Notched Geometries**  
: *Jeremy Massie<sup>1</sup>; Casey Holycross<sup>2</sup>; Joy Gockel<sup>1</sup>; <sup>1</sup>Wright State University; <sup>2</sup>Air Force Research Laboratory*

3:00 PM

**Obtaining High Strength-ductility Combination in Titanium by Microstructure and Texture Engineering through Multiaxial Plane-strain Forging:** *Devesh Chouhan<sup>1</sup>; Somjeet Biswas<sup>2</sup>; <sup>1</sup>Indian Institute of Technology KGP; <sup>2</sup>IIT KGP*

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**PROCESSING AND MANUFACTURING**

**Synthesis, Characterization, Modeling and Applications of Functional Porous Materials — Functional Porous Materials**

**Sponsored by:** ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Lan Li, Boise State University; Winnie Wong-Ng, National Institute of Standards and Technology; Kevin Huang, University of South Carolina

**Wednesday PM | October 20, 2021**  
**A212 | Greater Columbus Convention Center**

**Session Chairs:** Kevin Huang, University of South Carolina; Winnie Wong-Ng, National Institute of Standards and Technology (NIST)

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**2:00 PM Invited**

**Selected Pillared Cyanonickelate Based Metal Organic Frameworks (MOFs) for CO<sub>2</sub> Capture Applications:** *Winnie Wong-Ng<sup>1</sup>; Jeffrey Culp<sup>2</sup>; Yu-Sheng Chen<sup>3</sup>; Daniel Siderius<sup>1</sup>; Eric Cockayne<sup>2</sup>; Lan Li<sup>4</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>NETL; <sup>3</sup>University of Chicago; <sup>4</sup>Boise State University*

**2:30 PM Invited**

**Functional Applications of Porosity in Complex Crystals:** *Lawrence Cook<sup>1</sup>; Greg Brewer<sup>1</sup>; Winnie Wong-Ng<sup>2</sup>; Daniel Siderius<sup>2</sup>; <sup>1</sup>Catholic University of America; <sup>2</sup>National Institute of Standards and Technology*

**3:00 PM Invited**

**Porous Organic Polymer-based Nanotraps for Water Purification:** *Shengqian Ma<sup>1</sup>; <sup>1</sup>University of North Texas*

**3:30 PM Break**

**3:50 PM Invited**

**Recent Advances in High Temperature Multiphase Solid/Molten Carbonate Membranes for CO<sub>2</sub> Capture and Conversion:** *Kevin Huang<sup>1</sup>; <sup>1</sup>University of South Carolina*

**4:20 PM**

**Integrated Multi-characterization Approach to Understand Pore Size Distributions in Natural Porous Materials:** *V. V. Rohit Bukka<sup>1</sup>; Pankaj Sarin<sup>1</sup>; <sup>1</sup>Oklahoma State University*

**4:40 PM**

**Microporous Copper Spheres: Processing, Morphology, and Application:** *Braden Jones<sup>1</sup>; Beck Boan<sup>1</sup>; Mark Atwater<sup>1</sup>; <sup>1</sup>Liberty University*

Technical Meeting and Exhibition

# MS&T21

MATERIALS SCIENCE & TECHNOLOGY

October 17–20, 2021 | Columbus, Ohio

## POSTER SESSION WITH PRESENTERS

The poster sessions are divided into 3 separate presentation times and grouped by topic area. Poster presenters should stand by their poster during their designated presentation time.

### POSTER SESSION I

Tuesday, October 19  
11:00 a.m. to 12:00 p.m.

- Ceramic and Glass Materials
- Electronic and Magnetic Materials
- Fundamentals and Characterization
- Nanomaterials

### POSTER SESSION II

Tuesday, October 19  
12:00 p.m. to 1:00 p.m.

- Biomaterials
- Energy
- Materials-Environment Interactions
- Processing and Manufacturing

### POSTER SESSION III

Tuesday, October 19  
4:45 p.m. to 5:45 p.m.

- Additive Manufacturing
- Artificial Intelligence
- Iron and Steel (Ferrous Alloys)
- Modeling

## STUDENT EVENTS

### 2021 Undergraduate Student Poster Contest — 2021 Undergraduate Student Poster Contest

**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Effect of Carbon Stoichiometry on the Heat of Formation of Hafnium Carbides:** *Amelia Martinez<sup>1</sup>*; <sup>1</sup>Missouri University of Science and Technology

**Effect of Modifier Cation Size on the Bulk Structure and Nickel Speciation in Alkali Borosilicate Glasses:** *Lucas Greiner<sup>1</sup>*; Brian Topper<sup>1</sup>; Randall Youngman<sup>2</sup>; Doris Möncke<sup>1</sup>; <sup>1</sup>Alfred University; <sup>2</sup>Corning Inc.

**Enhanced Mechanical Properties in a 4140 Steel by "In-House" Intensive Quench:** *Larha Fernanda Vela<sup>1</sup>*; Jose Mariano Flores Herrera<sup>1</sup>; Simón de la Rosa de la Cruz<sup>1</sup>; Debanhi Ruvalcaba Quintero<sup>1</sup>; Abraham Escalona Gomez<sup>1</sup>; Jose Ivan López<sup>2</sup>; Moises Hinojosa Rivera<sup>1</sup>; <sup>1</sup>Universidad Autónoma de Nuevo León; <sup>2</sup>Metalsa

**Experiential Study on Critical Stress Intensity Factor of Carbon Nanotube Filled Epoxy:** *Lisa Zhou*; Yu Zhang<sup>1</sup>; Maobing Tu<sup>1</sup>; <sup>1</sup>University of Cincinnati

**Exploring the Liquid Phase Exfoliation of Two-Dimensional Bilayered Vanadium Oxide in Aqueous Media for Li ion Batteries:** *Raymond Zhang<sup>1</sup>*; Timofey Averianov<sup>1</sup>; Ekaterina Pomerantseva<sup>1</sup>; <sup>1</sup>Drexel University

**High Temperature Mechanical Properties of TiB<sub>2</sub>-WC-SiC Materials:** *Elizabeth Sayre<sup>1</sup>*; <sup>1</sup>Missouri University of Science and Technology

**Investigation of Embedded Metallic Components on 3D Printed Ceramic Structures:** *Victoria Adams<sup>1</sup>*; Eleanore Rogenski<sup>1</sup>; Bhargavi Mummareddy<sup>1</sup>; Eric MacDonald<sup>2</sup>; Pedro Cortes<sup>1</sup>; <sup>1</sup>Youngstown State University; <sup>2</sup>University of Texas at El Paso

**Machine Learning Approaches to Predict Properties from Microstructure Images in Ceramic-Metal Composites:** *Hugh Smith<sup>1</sup>*; William Huddleston<sup>1</sup>; Laura Bruckman<sup>1</sup>; Alp Sehirlioglu<sup>1</sup>; <sup>1</sup>Case Western Reserve University

**Mechanical Behavior of Automotive Structural Steels in the Vicinity of the Ductile-brittle Transition:** *Lesly Susana Briano Murillo<sup>1</sup>*; Moises Hinojosa Rivera<sup>1</sup>; <sup>1</sup>Universidad Autonoma de Nuevo León

**Perovskite Film Formation for Solar Cell Absorbers: Effects of Substrate Modification:** *Mirra Rasmussen*; Kyle Crowley<sup>1</sup>; Ina Martin<sup>1</sup>; <sup>1</sup>Case Western Reserve University

**Pressure Optimization of Fast-Moving Silicon MEMS Micromirrors:** *Adam Eichhorn<sup>1</sup>*; Andrew Oliver<sup>2</sup>; <sup>1</sup>Iowa State University; <sup>2</sup>Montana State University

**Processing and Properties of (Ta, Nb, Hf, Ti)C Reinforced with Carbon Fiber:** *Nathan Gillespie*

**Rheological Characterization of Highly Loaded Alumina-Polymer Suspension for Thermal Paste 3D Printing:** *Pattiya Pibulchinda<sup>1</sup>*; Caitlin Adams<sup>1</sup>; Kendra Erk<sup>1</sup>; <sup>1</sup>Purdue University School of Materials Engineering

**The Dynamic Performance of Wearable Sensors with Flexible Silver Ink:** *Gina Morrison<sup>1</sup>*; Charles Dwyer<sup>1</sup>; Gonzalo Carrillo<sup>2</sup>; Pedro Cortes<sup>1</sup>; Eric MacDonald<sup>3</sup>; <sup>1</sup>Youngstown State University; <sup>2</sup>Centro de Investigación Científica de Yucatán; <sup>3</sup>University of Texas at El Paso

**Thermal Analysis of Sodalite-immobilized Iodine-129 Caustic Scrubber Slurry:** *John Bussey<sup>1</sup>*; David Bollinger<sup>1</sup>; Jessica Erickson<sup>1</sup>; Natalie Smith-Gray<sup>1</sup>; John McCloy<sup>1</sup>; <sup>1</sup>Washington State University

**ZrB<sub>2</sub> Aqueous Slurry Development for DIW Additive Manufacturing:** *Elizabeth Malek<sup>1</sup>*; Connor Wyckoff<sup>1</sup>; James Kemp<sup>2</sup>; William Costakis<sup>2</sup>; Benjamin Lam<sup>2</sup>; Lisa Rueschhoff<sup>2</sup>; <sup>1</sup>Wright State University; <sup>2</sup>Air Force Research Lab

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advances in Dielectric Materials and Electronic Devices — Poster Session

**Sponsored by:** ACeRS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Ubic, Boise State University; Matjaž Spreitzer, Jožef Stefan Institute

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-11: Electric and Dielectric Characterization of [Cu, 2Ta] Dipole Substituted BaTiO<sub>3</sub> Ceramics:** *Noah Smith<sup>1</sup>*; Trisha Whaley<sup>1</sup>; Victoria Pellegrino<sup>1</sup>; Kaijie Ning<sup>1</sup>; Holly Shulman<sup>1</sup>; Walter Schulze<sup>1</sup>; Steven Tidrow<sup>1</sup>; <sup>1</sup>Alfred University

**P1-14: Nanoscale Dipole Engineered [Y, Ta] BaTiO<sub>3</sub> Ceramics For Relaxor-like Ferroelectrics:** *Victoria Pellegrino<sup>1</sup>*; Trisha Whaley<sup>1</sup>; Noah Smith<sup>1</sup>; Kaijie Ning<sup>1</sup>; Holly Shulman<sup>1</sup>; Walter Schulze<sup>1</sup>; Steven Tidrow<sup>1</sup>; <sup>1</sup>Alfred University

**P1-15: Novel Dipole-pair [Zn, W] Substituted BaTiO<sub>3</sub> Ceramic Relaxor:** *Trisha Whaley<sup>1</sup>*; Noah Smith<sup>1</sup>; Victoria Pellegrino<sup>1</sup>; Kaijie Ning<sup>1</sup>; Holly Shulman<sup>1</sup>; Walter Schulze<sup>1</sup>; Steven Tidrow<sup>1</sup>; <sup>1</sup>Alfred University

**P1-16: Observations from Testing Dielectric Elastomers in Uniaxial Tension:** *Carolyn Haase<sup>1</sup>*; Hector Medina<sup>1</sup>; <sup>1</sup>Liberty University

## CERAMIC AND GLASS MATERIALS

### Ceramic Matrix Composites — Poster Session

**Sponsored by:** ACeRS Engineering Ceramics Division

**Program Organizers:** Narottam Bansal, NASA Glenn Research Center; Jacques Lamon, CNRS; Sung Choi, Naval Air Systems Command

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chair:** Narottam Bansal, NASA Glenn Research Center

**P1-1: High Performance Oxide-Oxide CMCs:** *Logan Johnson<sup>1</sup>*; <sup>1</sup>Applied Thin Films, Inc.



# Technical Program

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## CERAMIC AND GLASS MATERIALS

### Ceramics and Glasses Modeling by Simulations and Machine Learning — Poster Session

**Sponsored by:** ACerS Glass & Optical Materials Division

**Program Organizers:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P1-3: Molecular Dynamic Characteristic Temperatures for Predicting Metallic Glass Forming Ability:** Lane Schultz<sup>1</sup>; Dane Morgan<sup>1</sup>; Izabela Szlufarska<sup>1</sup>; Benjamin Afflerbach<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

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## NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — Poster Session

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P1-31: Layered Metal Monochalcogenides as Electrodes for Electrochemical Energy Storage Applications:** Shakir Bin Mujib<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University

**P1-32: Low Temperature Synthesis of Solvothermally Grown Ga<sub>2</sub>O<sub>3</sub> Thin Films on FTO Substrates Enabling Various Functional Applications:** Siddhartha Suman<sup>1</sup>; Mukurula Nagaraju<sup>1</sup>; Lokanath Mohapatra<sup>1</sup>; Aditya Bhardwaj<sup>1</sup>; Ajay Kushwaha<sup>1</sup>; <sup>1</sup>Indian Institute of Technology

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## FUNDAMENTALS AND CHARACTERIZATION

### Deformation-induced Phase Transformations — Poster Session

**Program Organizers:** Yangyang Zhao, Purdue University; Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Janelle Wharry, Purdue University

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P1-18: Bimetallic Billets for Magnesium-thermal Production of High Quality Sponge Titanium:** Valeriy Mishchenko<sup>1</sup>; Svitlana Mudra<sup>1</sup>; Olha Bolsun<sup>1</sup>; Sergiy Sheyko<sup>1</sup>; <sup>1</sup>Zaporizhzhia National University

**P1-19: High-cut Steel Property Researches For Taps' Manufacture:** Anton Matiukhin<sup>1</sup>; Anna Ben<sup>1</sup>; Vitalii Shyrokobokov<sup>1</sup>; Sergey Sheyko<sup>1</sup>; Elena Kulabneva<sup>1</sup>; <sup>1</sup>"Zaporizhzhia Polytechnic" National University

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## FUNDAMENTALS AND CHARACTERIZATION

### Grain Boundaries, Interfaces, and Surfaces in Ceramics: Fundamental Structure—Property—Performance Relationships — Poster Session

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Rheinheimer Wolfgang, Forschungszentrum Jülich; Catherine Bishop, University of Canterbury; Shen Dillon, University of California, Irvine; Ming Tang, Rice University; John Blendell, Purdue University; Wayne Kaplan, Technion - Israel Institute of Technology; Melissa Santala, Oregon State University

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P1-20: A Novel Probe for Grain Boundary Characterization on the Mesoscopic Scale: Lab-based Diffraction Contrast Tomography:** Jun Sun<sup>1</sup>; Jette Oddershede<sup>1</sup>; Hrishikesh Bale<sup>2</sup>; Florian Bachmann<sup>1</sup>; William Harris<sup>3</sup>; Erik Lauridsen<sup>1</sup>; <sup>1</sup>Xnovo Technology; <sup>2</sup>Carl Zeiss X-ray Microscopy; <sup>3</sup>Carl Zeiss Microscopy, LLC

**P1-21: The Effect of High Energy Diffraction Microscopy (HEDM) and Laboratory Diffraction Contrast Tomography (LabDCT) Resolution on Measured Grain Growth Parameters in Strontium Titanate (SrTiO<sub>3</sub>):** Vivekanand Muralikrishnan<sup>1</sup>; Jette Oddershede<sup>2</sup>; He Liu<sup>3</sup>; Bryan Conry<sup>1</sup>; Florian Bachmann<sup>2</sup>; Robert Suter<sup>3</sup>; Amanda Krause<sup>1</sup>; <sup>1</sup>University of Florida; <sup>2</sup>Xnovo Technology ApS; <sup>3</sup>Carnegie Mellon University

## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III — Poster Session

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-22: Life Prediction of High Temperature Alloys Subject to Coupled Thermomechanical Fatigue-creep Condition:** *Abhilash Gulhane*<sup>1</sup>; Harshal Dhamade<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

## SPECIAL TOPICS

### Late News Poster Session — Ceramic and Glass Materials

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-5: Oxidation Protection of AlN/BN via  $Al_{18}B_4O_{33}$ :** *Celia Chari*<sup>1</sup>; Katherine Faber<sup>1</sup>; <sup>1</sup>California Institute of Technology

**P1-6: Luminescence Thermometry – a Fad or a Challenge?:** *Malgorzata Sójka*<sup>1</sup>; Marcin Runowski<sup>2</sup>; Przemysław Wozny<sup>2</sup>; Luis Carlos<sup>3</sup>; Eugeniusz Zych<sup>1</sup>; Stefan Lis<sup>2</sup>; <sup>1</sup>University of Wrocław; <sup>2</sup>Adam Mickiewicz University; <sup>3</sup>University of Aveiro

**P1-7: Preparation and Structural Evolution of Si(O)CN Fibers Prepared via Hand Spinning of a Modified Silazane Oligomer:** *Ellie Christman*<sup>1</sup>; Christel Gervais<sup>2</sup>; Gurpreet Singh<sup>3</sup>; Himanshu Jain<sup>1</sup>; <sup>1</sup>Lehigh University; <sup>2</sup>Sorbonne University; <sup>3</sup>Kansas State University

## SPECIAL TOPICS

### Late News Poster Session — Electronic and Magnetic Materials

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-17: Hydrogen Induced Photodarkening of Cu-doped B-Ga2O3 Czochralski Single Crystals:** *Jani Jesenovec*<sup>1</sup>; Christopher Pansegrau<sup>1</sup>; Cassandra Remple<sup>1</sup>; Jesse Huso<sup>2</sup>; Matthew McCluskey<sup>1</sup>; John McCloy<sup>1</sup>; <sup>1</sup>Washington State University; <sup>2</sup>Klar Scientific

## SPECIAL TOPICS

### Late News Poster Session — Fundamentals and Characterization

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-27: Polyurea Tensile Tests at High Strain Rates:** *Frederick Heim*<sup>1</sup>; Sidney Chocron<sup>1</sup>; Arthur Nicholls<sup>1</sup>; Lynsey Reese<sup>2</sup>; <sup>1</sup>Southwest Research Institute; <sup>2</sup>US Navy NAVFAC

## SPECIAL TOPICS

### Late News Poster Session — Nanomaterials

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-34: Resilient SiOC/Epoxy Nanocomposites:** *Tulsi Patel*<sup>1</sup>; Robert Wheeler<sup>1</sup>; Derek King<sup>1</sup>; Andrew Sharits<sup>1</sup>; Ryan Nielsen<sup>2</sup>; Pania Newell<sup>2</sup>; Lisa Rueschhoff<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>University of Utah

**P1-35: Spectroscopic Studies of Nd3+ Doped KY3F10 Nanoparticles:** *Sangeetha Balabhadra*<sup>1</sup>; Michael Reid<sup>1</sup>; Jon-Paul Wells<sup>1</sup>; <sup>1</sup>University of Canterbury

## FUNDAMENTALS AND CHARACTERIZATION

### Nucleation of Solid-State Phase Transformations — Poster Session

**Sponsored by:** TMS Phase Transformations Committee

**Program Organizers:** Eric Lass, University of Tennessee-Knoxville; Sophie Primig, University of New South Wales; Keith Knipling, Naval Research Laboratory

**11:00 AM to 12:00 PM**  
**Tuesday AM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P1-28: Structure Influenced Rapid Hydrogenation Using Metal-acid Contacts on Crystallographically Oriented VO2 Thin Films:** *Komal Mulchandani*<sup>1</sup>; Ankit Soni<sup>2</sup>; Krushna Mavani<sup>3</sup>; <sup>1</sup>Indian Institute of Technology Indore, Rajeev Gandhi Govt. P. G. College, Mandsaur (M.P.); <sup>2</sup>Indian Institute of Technology Delhi; <sup>3</sup>Indian Institute of Technology Indore

# Technical Program

## CERAMIC AND GLASS MATERIALS

### Phase Transformations in Ceramics: Science and Applications — Poster Session

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Scott McCormack, University of California, Davis; Pankaj Sarin, Oklahoma State University; Sanjay V. Khare, University of Toledo; Waltraud Kriven, University of Illinois at Urbana-Champaign

**11:00 AM to 12:00 PM**

**Tuesday AM | October 19, 2021**

**Exhibit Hall B | Greater Columbus Convention Center**

**P1-8: Structure, Electronic and Optical Properties of Ternary Nitride Phases of  $\text{MgSnN}_2$ : A First-principles Study:** *Bishal Dumre*<sup>1</sup>; Daniel Gall<sup>2</sup>; Sanjay Khare<sup>1</sup>; <sup>1</sup>The University of Toledo; <sup>2</sup>Rensselaer Polytechnic Institute

**P1-9: Understanding the Effect of Aliovalent Doping on Phase Transformations and Thermo-physical Properties in  $\text{RENbO}_4$ :** Daniel Lowry<sup>1</sup>; *Pankaj Sarin*<sup>1</sup>; <sup>1</sup>Oklahoma State University

## FUNDAMENTALS AND CHARACTERIZATION

### Processing—Microstructure—Property Relationships of Titanium and Titanium Alloys — Poster Session

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Yufeng Zheng, University of Nevada-Reno; Rongpei Shi, Lawrence Livermore National Laboratory; Michael Gram, Titanium Metals Corporation

**11:00 AM to 12:00 PM**

**Tuesday AM | October 19, 2021**

**Exhibit Hall B | Greater Columbus Convention Center**

**P1-29: Hierarchical Twinning Microstructure in the Metastable  $\beta$  Ti-24Nb-4Zr-8Sn Alloy:** *Wenrui Zhao*<sup>1</sup>; Dian Li<sup>1</sup>; Yufeng Zheng<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

**P1-30: Analysis of Temperature Factor Influence on the Nature of the Titanium Alloy Deformation during Extrusion:** *Anton Matiukhin*<sup>1</sup>; Anna Ben<sup>1</sup>; Vitalii Shyrokobokov<sup>1</sup>; Sergey Sheyko<sup>1</sup>; Elena Kulabneva<sup>1</sup>; <sup>1</sup>"Zaporizhzhia Polytechnic" National University

## PROCESSING AND MANUFACTURING

### 13th Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing — Poster Session

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Surojit Gupta, University of North Dakota; Rajiv Asthana, University of Wisconsin; Hisayuki Suematsu, Nagaoka University of Technology; Mritunjay Singh, Ohio Aerospace Institute; Enrico Bernardo, University of Padova; Yiquan Wu, Alfred University; Zhengyi Fu, Wuhan University of Technology; Allen Apblett, Oklahoma State University; Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology

**12:00 PM to 1:00 PM**

**Tuesday PM | October 19, 2021**

**Exhibit Hall B | Greater Columbus Convention Center**

**P2-20: Biomass Derived  $\text{SiO}_2$ : Different Waste Resources and Extraction Methods:** *Damandeep Kaur*<sup>1</sup>; O.P. Pandey<sup>1</sup>; M.S. Reddy<sup>1</sup>; <sup>1</sup>Thapar Institute of Engineering & Technology

**P2-21: Effect of Steam Injection on Reduction of Dioxin Emission from the Commercial-scale Sintering Plant:** *Zhengyun Fan*<sup>1</sup>; Wen Pan<sup>1</sup>; Shiqi Zhao<sup>1</sup>; <sup>1</sup>Shougang Research Institute of Technology

**P2-22: Metallurgical Quality Analysis of High Nb TiAl Alloy Cast Ingot Prepared by BaZrO<sub>3</sub> Crucible:** *Xuexian Zhang*<sup>1</sup>; Guangyao Chen<sup>1</sup>; Bao Hua Duan<sup>1</sup>; Yuchen Yang<sup>1</sup>; <sup>1</sup>Shanghai University

**P2-23: Optimization of the Ratio of Air and Fuel in Ignition Chamber of Sintering Machine:** *Yapeng Zhang*<sup>1</sup>; Wen Pan<sup>1</sup>; Jingjun Zhao<sup>2</sup>; Shaoguo Chen<sup>1</sup>; Huaiying Ma<sup>1</sup>; Zhixing Zhao<sup>1</sup>; <sup>1</sup>Research Institute of Iron & Steel, Shougang Group Co., LTD Research Institute of Technology; <sup>2</sup>Ironmaking Department, Shougang Jingtang United Iron & Steel Co., Ltd

**P2-24: Research on West Pilbara Fines (WPF) Utilization under Deep Bed Sintering:** *Wen Pan*<sup>1</sup>; Shaoguo Chen<sup>1</sup>; Yapeng Zhang<sup>1</sup>; <sup>1</sup>Research Institute of Iron & Steel, Shougang Group Co., LTD Research Institute of Technology

**P2-25: Reform and Practice of Energy Saving and Consumption Reduction Technology of 500 t/d Beckenbach Annular Lime Kiln:** *Yapeng Zhang*<sup>1</sup>; Wen Pan<sup>2</sup>; Zhenping Miao<sup>1</sup>; Shaoguo Chen<sup>2</sup>; Huaiying Ma<sup>2</sup>; Zhixing Zhao<sup>2</sup>; <sup>1</sup>Shougang Group; <sup>2</sup>Research Institute of Iron & Steel, Shougang Group Co., LTD Research Institute of Technology

**P2-26: Study on Application of King Ore Fines in Sintering Process of Shougang Jingtang Plant:** *Shaoguo Chen*<sup>1</sup>; Wen Pan<sup>1</sup>; Yapeng Zhang<sup>1</sup>; Xiaochen Zhang<sup>1</sup>; Bin Ji<sup>1</sup>; Zhixing Zhao<sup>1</sup>; <sup>1</sup>Shougang Research Institute of Technology

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Coatings for Wear and Corrosion Protection — Poster Session

**Program Organizers:** Evelina Vogli, Lm Group Holdings Inc.; Virendra Singh, Schlumberger

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chair:** Evelina Vogli, LM Group Holdings

**P2-12: Increase of Wearproofness Steel Surface as a Result Mechanochemical Influence Polymethylmethacrylate:** Volodymyr Tsyganov<sup>1</sup>; <sup>1</sup>"Zaporizhzhia Polytechnic" National University

**P2-13: Increased Efficiency Surface Diffusion Metalization of Cast Iron and Steel Chemical Equipment Parts:** Svetlana Kondrashova<sup>1</sup>; Egor Saprykin<sup>1</sup>; Valeriy Naumyk<sup>2</sup>; Sergey Sheyko<sup>3</sup>; <sup>1</sup>Berdiansk Mechanical Engineering College of National University "Zaporizhzhia Polytechnic"; <sup>2</sup>NU "Zaporizhzhia Polytechnic"; <sup>3</sup>Zaporizhzhia National University

**P2-14: Production Aluminized Alloyed Coatings for Protection Against Wear and Corrosion:** Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Irina Kruglyak<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University

## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — Poster Session

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P2-16: Development of Porous Silicon Nitride for Hypersonic RF Window Applications:** Averyonna Kimery<sup>1</sup>; <sup>1</sup>Purdue University

## PROCESSING AND MANUFACTURING

### Advances in Surface Engineering — Poster Session

**Sponsored by:** TMS Surface Engineering Committee

**Program Organizers:** Rajeswaran Radhakrishnan, Faraday Technology Inc; Brian Skinn, Faraday Technology, Inc.; Timothy Hall, Faraday Technology Inc; Michael Roach, University of Mississippi Medical Center; Sandip Harimkar, Oklahoma State University; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chair:** Rajeswaran Radhakrishnan, Faraday Technology Inc

**P2-27: Novel Rosette-like Formations on Ti Surfaces with Nanosize "Petal" Features:** Hector Medina<sup>1</sup>; <sup>1</sup>Liberty University

## MATERIALS-ENVIRONMENT INTERACTIONS

### Computation Assisted Materials Development for Improved Corrosion Resistance — Poster Session

**Program Organizers:** Rishi Pillai, Oak Ridge National Laboratory; Laurence Marks, Northwestern University

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P2-17: Development of Rhenium Free Heat-resistant Nickel Alloy for the Cast Blades Production by the Method of Directional Crystallization:** Evgeniy Milonin<sup>1</sup>; Konstantin Balushok<sup>1</sup>; Pavel Malinovsky<sup>1</sup>; Valeriy Naumyk<sup>2</sup>; Vadim Shalomeev<sup>2</sup>; Sergey Sheyko<sup>3</sup>; <sup>1</sup>JSC «Motor Sich»; <sup>2</sup>NU "Zaporizhzhia Polytechnic"; <sup>3</sup>Zaporizhzhia National University

## SPECIAL TOPICS

### Late News Poster Session — Biomaterials

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P2-2: Effect of Copolyolysis on the Composition of Soursop (Annona Muricata) and Mango (Mangifera Indica) Seeds Bio-oil:** Esther Ikhuoria<sup>1</sup>; Joshua Onaifo<sup>1</sup>; <sup>1</sup>University of Benin



# Technical Program

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## SPECIAL TOPICS

### Late News Poster Session — Energy

12:00 PM to 1:00 PM  
Tuesday PM | October 19, 2021  
Exhibit Hall B | Greater Columbus Convention Center

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**P2-9: Computational Fluid Dynamics Modeling of Enhanced Convective Heat Transfer Using Twisted Tape Insert:** *Kshitija Kshitija<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jian Zhang<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis*

**P2-10: Correlation between Shear Strength and PU Foam Density with Respect to Aging Time in District Heating Pipe:** *Hyung-Gyu Kim<sup>1</sup>; Jaehoon Park<sup>1</sup>; Jooyong Kim<sup>2</sup>; Hae-Yong Lee<sup>2</sup>; Jonghun Yoon<sup>1</sup>; <sup>1</sup>Hanyang University; <sup>2</sup>Korea District Heating Corporation (KDHC)/Frontier Research & Training Institute*

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## SPECIAL TOPICS

### Late News Poster Session — Processing and Manufacturing

12:00 PM to 1:00 PM  
Tuesday PM | October 19, 2021  
Exhibit Hall B | Greater Columbus Convention Center

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**P2-29: Porous Metal Micro-pillars by Thermomechanical Molding:** *Shweta Jagdale<sup>1</sup>; Golden Kumar<sup>1</sup>; <sup>1</sup>University of Texas at Dallas*

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## BIOMATERIALS

### Next Generation Biomaterials — Poster Session

*Sponsored by:* ACerS Bioceramics Division, TMS Biomaterials Committee

*Program Organizers:* Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

12:00 PM to 1:00 PM  
Tuesday PM | October 19, 2021  
Exhibit Hall B | Greater Columbus Convention Center

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**P2-3: Stretchable Ion Responsive Hydrogel with Controlled Response:** *Abhishek Pachauri<sup>1</sup>; Jeff Bates<sup>1</sup>; <sup>1</sup>University of Utah*

**P2-4: A Skin Testing Diagnostic Device:** *Anthony Annerino<sup>1</sup>; Pelagia-Iren Gouma<sup>1</sup>; <sup>1</sup>The Ohio State University*

**P2-6: Non-clinical Method For Diagnosing Cystic Fibrosis:** *Cassidy Holdeman<sup>1</sup>; <sup>1</sup>University of Utah*

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## BIOMATERIALS

### Porous Materials for Biomedical Applications — Poster Session

*Sponsored by:* ACerS Bioceramics Division

*Program Organizers:* Usman Liaqat, National University of Sciences and Technology; Chuanbin Mao, University of Oklahoma; Mingying Yang, Zhejiang University

12:00 PM to 1:00 PM  
Tuesday PM | October 19, 2021  
Exhibit Hall B | Greater Columbus Convention Center

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**P2-7: 3D Printing Seamless Hydrogels for In-vivo Pressure Sensing Devices:** *Ashwin Velraj<sup>1</sup>; Jeffrey Bates<sup>1</sup>; <sup>1</sup>University of Utah*

**P2-8: In vitro Investigation and Characterization of Resorption and Degradation Behavior of X-Ca-alginate Aerogels for Tissue Scaffold Applications:** *Martina Rodriguez Sala<sup>1</sup>; Grigorios Raptopoulos<sup>2</sup>; Patrino Paraskevopoulou<sup>2</sup>; Firouzeh Sabri<sup>1</sup>; <sup>1</sup>The University of Memphis; <sup>2</sup>National and Kapodistrian University of Athens*

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## PROCESSING AND MANUFACTURING

### Synthesis, Characterization, Modeling and Applications of Functional Porous Materials — Poster Session

*Sponsored by:* ACerS Electronics Division, ACerS Engineering Ceramics Division

*Program Organizers:* Lan Li, Boise State University; Winnie Wong-Ng, National Institute of Standards and Technology; Kevin Huang, University of South Carolina

12:00 PM to 1:00 PM  
Tuesday PM | October 19, 2021  
Exhibit Hall B | Greater Columbus Convention Center

*Session Chair:* Lan Li, Boise State University

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**P2-30: ScSZ-MC Dual-phase Tubular Membrane for Pre-combustion CO<sub>2</sub> Capture:** *Shichen Sun<sup>1</sup>; Kevin Huang<sup>1</sup>; <sup>1</sup>University of South Carolina*

**P2-31: Geopolymer Adsorbents for Harvesting N and P from Poultry Litter:** *Gizem Topal<sup>1</sup>; Pankaj Sarin<sup>1</sup>; V.V. Rohit Bukka<sup>1</sup>; <sup>1</sup>Oklahoma State University*

## MATERIALS-ENVIRONMENT INTERACTIONS

### Thermodynamics of Materials in Extreme Environments — Poster Session

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division

**Program Organizers:** Xiaofeng Guo, Washington State University; Kristina Lilova, Arizona State University; Kyle Brinkman, Clemson University; Alexandra Navrotsky, Arizona State University; Jake Amoroso, Savannah River National Laboratory; Xingbo Liu, West Virginia University; Gustavo Costa, NASA Glenn Research Center

**12:00 PM to 1:00 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chairs:** Kristina Lilova, Arizona State University; Xiaofeng Guo, Washington State University

**P2-19: Design of Ultra-high Temperature Ceramics for Oxidation Resistance:** *Niquana S<sup>1</sup>*; Elizabeth Opila Opila<sup>1</sup>; <sup>1</sup>University of Virginia

## ARTIFICIAL INTELLIGENCE

### Accelerating Materials Science with Big Data and Machine Learning — Poster Session

**Program Organizers:** Huan Tran, Georgia Institute of Technology; Muratahan Aykol, Toyota Research Institute

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**P3-18: Rashba Spin Splitting and Photocatalytic Properties of GeC-MSSe (M=Mo, W) Van Der Waals Heterostructures:** *Haleem Ud Din<sup>1</sup>*; <sup>1</sup>Abbottabad University of Science & Technology

**P3-19: Thermo-mechanical Property Prediction of High-temperature Materials Using a Python Based Interface With Quantum Espresso:** *Joseph Derrick<sup>1</sup>*; Michael Golub<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — Poster Session

**Sponsored by:** TMS Computational Materials Science and Engineering Committee

**Program Organizers:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chair:** Jing Zhang, Indiana University – Purdue University Indianapolis

**P3-1: Creep Modeling of 3D Printed Nickel Based Superalloy:** *Harshal Dhamade<sup>1</sup>*; Abhilash Gulhane<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

**P3-2: Design A Syringe Pump Extruder Type 3D Bioprinter:** *Haoyee Yeong<sup>1</sup>*; Eli Kindomba<sup>1</sup>; Bavly Shehata<sup>1</sup>; Alyaa Idris<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

**P3-3: Finite Element Modeling of Coating Thickness Prediction in Electron Beam Physical Vapor Deposition Process:** *Anvesh Dhulipalla<sup>1</sup>*; Yafeng Li<sup>2</sup>; Sugrim Sagar<sup>1</sup>; Jian Zhang<sup>1</sup>; Xuehui Yang<sup>1</sup>; Dan Koo<sup>1</sup>; Hye-Yeong Park<sup>3</sup>; Yeon-Gil Jung<sup>3</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis; <sup>2</sup>Tiangong University; <sup>3</sup>Changwon National University

**P3-4: Modeling Charpy Impact Property of 3D Printed 718 Nickel Alloys Using the Smoothed Particle Hydrodynamics Method:** *Sugrim Sagar<sup>1</sup>*; Jian Zhang<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

**P3-5: Reinforcement Learning Aided Simulations for Determining Process Parameters for Optimizing Microstructure in LPBF Additive Manufacturing Parts:** *Junwon Seo<sup>1</sup>*; Joseph Pauza<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**P3-6: Student Design Project of Design a Mechanical Ventilator Prototype during the Pandemic:** *Francis Iloeje<sup>1</sup>*; Sunday Folorunso<sup>1</sup>; Haoyee Yeong<sup>1</sup>; Eli Kindomba<sup>1</sup>; Yafeng Li<sup>2</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis; <sup>2</sup>Tiangong University

**P3-7: Virtual Reality Modules of 3D Printing Laboratories for Additive Manufacturing Education:** *Cooper Zuranski<sup>1</sup>*; Shambhuraj Wadghule<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — Poster Session

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P3-9: Characterization of Stresses as a Function of AM Processing Parameters in Commercially Pure Ti:** *Claire Adams<sup>1</sup>; Kellen Traxel<sup>1</sup>; Amit Bandyopadhyay<sup>1</sup>; David Field<sup>1</sup>; <sup>1</sup>Washington State University*

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## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Metallic Coated Advanced Steels — Poster Session

**Sponsored by:** AIST: Metallurgy Processing Products and Applications Technology Committee, AIST: Galvanizing Technology Committee

**Program Organizers:** Joseph McDermid, McMaster University; Frank Goodwin, ILZRO

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

**Session Chair:** Frank Goodwin, International Zinc Association

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**P3-22: Reduction of the Internal and External Oxidation of the Charge during Galvanizing Under SHS Conditions:** *Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Irina Kruglyak<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University*

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## SPECIAL TOPICS

### Late News Poster Session — Additive Manufacturing

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P3-10: Additively Manufactured 718 Ni Alloys with Oxide Nanoparticles:** *Benjamin Stegman<sup>1</sup>; Xinghang Zhang<sup>1</sup>; Haiyan Wang<sup>1</sup>; Bo Yang<sup>1</sup>; Zhongxia Shang<sup>1</sup>; Jie Ding<sup>1</sup>; Tianyi Sun<sup>1</sup>; William Jarosinski<sup>1</sup>; Jack Lopez<sup>1</sup>; <sup>1</sup>Purdue University*

**P3-11: CALPHAD-based Alloy Design and Uncertainty Quantification for Additive Manufacturing:** *Xin Wang<sup>1</sup>; Soumya Sridar<sup>1</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**P3-13: Effect of Heat Treatment on Microstructure and Corrosion Behavior of Additively Manufactured 7050 Aluminum Alloy:** *Rupesh Rajendran<sup>1</sup>; Preet Singh<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology*

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## SPECIAL TOPICS

### Late News Poster Session — Iron and Steel (Ferrous Alloys)

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P3-26: Introducing Heusler Fe<sub>3</sub>SiTi Intermetallic as a New Strengthening Precipitate for High Strength Low Alloy Steels:** *Rafael Rodriguez De Vecchis<sup>1</sup>; Xin Wang<sup>1</sup>; Soumya Sridar<sup>1</sup>; Zhangwei Wang<sup>2</sup>; Wei Xiong<sup>1</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH*

**P3-27: Understanding the Load Response Behavior of Martensite, Bainite and Accompanied Retained Austenite in a High Carbon Bearing Steel:** *Mohanchand Paladugu<sup>1</sup>; Daniel Foster<sup>2</sup>; Enrique Jimenez-melero<sup>2</sup>; Lee M. Rothleutner<sup>1</sup>; R. Scott Hyde<sup>1</sup>; <sup>1</sup>The Timken Company World Headquarters (WHQ), North Canton, OH 44720, USA; <sup>2</sup>Materials Performance Centre, Department of Materials, The University of Manchester, UK*

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## SPECIAL TOPICS

### Late News Poster Session — Modeling

**4:45 PM to 5:45 PM**  
**Tuesday PM | October 19, 2021**  
**Exhibit Hall B | Greater Columbus Convention Center**

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**P3-28: Fatigue Analysis of a Spring Coil Structure under Cyclic Loading Conditions:** *Sunday Folorunso<sup>1</sup>; Jian Zhang<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis*

**P3-29: Finite Element Modeling of Sheet Metal Bending Process:** *Sunket Kulkarni<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jian Zhang<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis*

**P3-30: Grain Size-texture Coupling in Crystal Plasticity Finite Element Modeling : Application to Magnesium Alloys:** *Aaditya Lakshmanan<sup>1</sup>; Mohsen Andani<sup>1</sup>; Veera Sundararaghavan<sup>1</sup>; Amit Misra<sup>1</sup>; John Allison<sup>1</sup>; <sup>1</sup>University Of Michigan*

**P3-31: Reactive Phase Formation: Kinetics and Associated Microstructure Evolution:** *Connor McNamara<sup>1</sup>; Helen Chan<sup>1</sup>; Jeffrey Rickman<sup>1</sup>; <sup>1</sup>Lehigh University*

**P3-32: Understanding Mechanical Behavior of Basketball Hoops Using Finite Element Modeling:** *Luc Rulinda<sup>1</sup>; Jian Zhang<sup>1</sup>; Tejesh Dube<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis*

Technical Meeting and Exhibition

# MS&T21

MATERIALS SCIENCE & TECHNOLOGY

**October 17–20, 2021 | Columbus, Ohio**

## **ON-DEMAND PRESENTATIONS**

The following are details to help prepare for the program if you are presenting in the virtual on-demand option:

- The on-demand presentations are scheduled to be available beginning Friday, October 22 starting at 8:00 a.m. EDT.
- The presentations will be available to view through December 31, 2021.
- Presentations will be pre-recorded.
- All presentations and events will be scheduled in Eastern Daylight Time (UTC-4:00).



# Technical Program

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## PROCESSING AND MANUFACTURING

### 13th Symposium on Green and Sustainable Technologies for Materials Manufacturing and Processing — On-Demand Novel Approaches to Sustainable Manufacturing

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Surojit Gupta, University of North Dakota; Rajiv Asthana, University of Wisconsin; Hisayuki Suematsu, Nagaoka University of Technology; Mritunjay Singh, Ohio Aerospace Institute; Enrico Bernardo, University of Padova; Yiquan Wu, Alfred University; Zhengyi Fu, Wuhan University of Technology; Allen Apblett, Oklahoma State University; Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 12 | MS&T On Demand**

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#### Invited

**Sustainable Processing of Composite Materials:** *Daniel Kopp*<sup>1</sup>; Kevin Blinn<sup>2</sup>; Jun Wang<sup>2</sup>; Daniel McMullen<sup>2</sup>; Surojit Gupta<sup>3</sup>; Richard Riman<sup>1</sup>; <sup>1</sup>Rutgers University; <sup>2</sup>RRTC Inc.; <sup>3</sup>University of North Dakota

#### Invited

**Gelation-freezing Derived Mullite Thermal Insulators Prepared by Reaction Sintering with Various Types of Alumina Nanofibers and Silica:** *Manabu Fukushima*<sup>1</sup>; <sup>1</sup>National Institute of Advanced Industrial Science and Technology

#### Invited

**Addressing Advanced Sustainability with Materials Selection:** *Luca Masì*<sup>1</sup>; Mauricio Dwek<sup>1</sup>; <sup>1</sup>Ansys Inc.

#### Invited

**Sustainable Synthesis of Non-oxide Ceramics in Air:** *Jesus Gonzalez-Julian*<sup>1</sup>; Apurv Dash<sup>1</sup>; Sylvain Badier<sup>1</sup>; Robert Vassen<sup>1</sup>; Olivier Guillon<sup>1</sup>; <sup>1</sup>Forschungszentrum Jülich

#### Invited

**Preparation of Tin Nanosized Powder by Pulsed Wire Discharge:** *Hisayuki Suematsu*<sup>1</sup>; Souma Yamamoto<sup>1</sup>; Thi Do<sup>1</sup>; Tadachika Nakayama<sup>1</sup>; <sup>1</sup>Nagaoka University of Technology

#### Invited

**Room-temperature Densification of MgO Ceramics with Nitride Phosphor Particles:** *Junichi Tatami*<sup>1</sup>; Emi Takahashi<sup>1</sup>; Takuma Takahashi<sup>1</sup>; <sup>1</sup>Yokohama National University

#### Invited

**Smart Powder Processing for Sustainable Society:** *Makio Naito*<sup>1</sup>; Takahiro Kozawa<sup>1</sup>; Akira Kondo<sup>1</sup>; <sup>1</sup>Osaka University

#### Invited

**Polymer Derived Coatings for Corrosion Protection of Steels:** *Kathy Lu*<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University

#### Invited

**First-principles Studies of Adsorption and Diffusion of Metal on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> for Advanced Manufacturing Applications:** *Austin Biagagne*<sup>1</sup>; Lan Li<sup>1</sup>; <sup>1</sup>Boise State University

#### Invited

**The Printability of Ternary Metal Boride (MAB) Materials Using Laser Powder Bed Fusion:** *Samuel Hocker*<sup>1</sup>; Mackenzie Geigle<sup>2</sup>; Taylor Riedl<sup>2</sup>; Christian Forsberg<sup>2</sup>; Maharshi Dey<sup>2</sup>; Karen Taminger<sup>1</sup>; Lopamudra Das<sup>3</sup>; Surojit Gupta<sup>2</sup>; Valerie Wiesner<sup>1</sup>; Daniel Trieff<sup>2</sup>; <sup>1</sup>NASA Langley Research Center; <sup>2</sup>University of North Dakota; <sup>3</sup>National Institute of Aerospace

**High Temperature Interaction of IN718 on Heated Buildplate:** *Nicolas Tan*<sup>1</sup>; <sup>1</sup>University of Arizona

**Preparation of BaZrO<sub>3</sub>/Y<sub>2</sub>O<sub>3</sub> Composite Refractory and Study on Its Interface Reaction with Ti<sub>2</sub>Ni Alloy:** *Xiao Hou*<sup>1</sup>; Feihai Yu<sup>1</sup>; Yucheng Yang<sup>1</sup>; Guangyao Chen<sup>1</sup>; <sup>1</sup>Shanghai University

**Study on the Interfacial Reaction between BaZrO<sub>3</sub> Refractories and Zr Amorphous Alloys:** *Feihai Yu*<sup>1</sup>; Guangyao Chen<sup>1</sup>; Xiao Hou<sup>1</sup>; Yuchen Yang<sup>1</sup>; Chonghe Li<sup>1</sup>; <sup>1</sup>Shanghai University

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## STUDENT EVENTS

### 2021 Undergraduate Student Poster Contest — On-Demand Poster Presentations

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Composition and Physicochemical Properties of Typical Waste Cooking Oil:** Qingyao Yu<sup>1</sup>; Peng Li<sup>1</sup>; Jing Wu<sup>2</sup>; *Xiaofeng Cheng*<sup>3</sup>; Gui-xia Fan<sup>1</sup>; <sup>1</sup>Zhengzhou University; <sup>2</sup>Huaibei Blasting Technology Research Institute Co.,Ltd.,CCTEG; <sup>3</sup>Zhengzhou Institute of Multipurpose Utilization of Mineral Resources, CAGS

**Electron Cloud Migration Effect-induced Lithiophobicity/Lithiophilicity Transformation for Dendrite-free Lithium Metal Anodes:** *Qianqiao Li*<sup>1</sup>; <sup>1</sup>Wuhan University of Technology

**Highly Crystallized Prussian Blue with Enhanced Kinetics for Highly Efficient Sodium Storage:** *Ruixuan Jiang*<sup>1</sup>; Mingsheng Qin<sup>2</sup>; <sup>1</sup>Wuhan University of Technology; <sup>2</sup>Huazhong University of Science and Technology

**Mechanical Property Assessment of Silicon Carbide Fiber-reinforced Epoxy-matrix Composites:** *Dylan Kruep*<sup>1</sup>; Shakir Bin Mujib<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University

**Optimal Integration of TiO<sub>2</sub>-Coated Gold Nanostars for Enhancement of Photocatalytic Water Reduction:** *Sanjna Sukumaran*<sup>1</sup>; Kaleigh Ryan<sup>1</sup>; Laura Fabris<sup>1</sup>; <sup>1</sup>Rutgers University

**The Mechanisms of Micro-fine Titanogite Enter to Ilmenite in the Flotation and Depression Behavior of Sodium Silicate:** Gui-xia Fan<sup>1</sup>; Xiaofeng Cheng<sup>2</sup>; Jing Wu<sup>3</sup>; Peng Li<sup>1</sup>; <sup>1</sup>Zhengzhou University; <sup>2</sup>Zhengzhou Institute of Multipurpose Utilization of Mineral Resources, CAGS; <sup>3</sup>Huaibei Blasting Technology Research Institute Co.,Ltd.,CCTEG

## ARTIFICIAL INTELLIGENCE

### Accelerating Materials Science with Big Data and Machine Learning — On-Demand Oral Presentations

**Program Organizers:** Huan Tran, Georgia Institute of Technology; Muratahan Aykol, Toyota Research Institute

**Friday AM | October 22, 2021**  
**On-Demand Room 2 | MS&T On Demand**

#### Invited

**Bridging the Gap between Literature Data Extraction and Domain Specific Materials Informatics:** *Elsa Olivetti*<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

#### Invited

**There is No Time for Science as Usual:** *Alan Aspuru-Guzik*<sup>1</sup>; <sup>1</sup>University of Toronto

#### Invited

**Designing Alloys with Process-mapping AI Pre-trained on Empirical Knowledge:** *Vyacheslav Romanov*<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

#### Invited

**Accelerating Discovery in Computational Materials Science Using CAMD:** *Joseph Montoya*<sup>1</sup>; <sup>1</sup>Toyota Research Institute

**Scalable Gaussian Processes for Predicting the Optical, Physical, Thermal, and Mechanical Properties of Inorganic Glasses Using Compositions for Large Datasets:** *Suresh Bishnoi*<sup>1</sup>; Ravinder Ravinder<sup>1</sup>; Hargun Singh Grover<sup>1</sup>; Hariprasad Kodamana<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology, Delhi

**Deep Learning-enabled Prediction of Mechanical Properties of Metallic Microlattice Structures Using Uniaxial Compression Videos:** *Akanksh Shetty*<sup>1</sup>; Chunshan Hu<sup>1</sup>; Mohammad Sadeq Saleh<sup>1</sup>; Jack Beuth<sup>1</sup>; Rahul Panat<sup>1</sup>; Amir Farimani<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

**Molecular Dynamics Simulation Using Lagrangian Neural Networks:** *Ravinder Bhattoo*<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi

**Multi-target Prediction of Concrete Engineering Properties Based on a Single Deep Learning Model:** *Yu Song*<sup>1</sup>; Gaurav Sant<sup>1</sup>; Mathieu Bauchy<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

**Semantic Segmentation of Plasma Transferred Arc Additively Manufactured NiBSi-WC Optical Microscopy Images Using a Convolutional Neural Network:** *Dylan Rose*<sup>1</sup>; Justin Forth<sup>2</sup>; Tonya Wolfe<sup>3</sup>; Ahmed Qureshi<sup>1</sup>; Hani Henein<sup>1</sup>; <sup>1</sup>University of Alberta; <sup>2</sup>Consultant; <sup>3</sup>Red Deer College

**Machine Learning in 2D Materials: Benchmarking Crystal Graph Based Convolutional Neural Network (CGCNN) for Open Databases:** *Shreeja Das*<sup>1</sup>; Raj Kishore<sup>1</sup>; Mihir Sahoo<sup>1</sup>; S Swayamjyoti<sup>1</sup>; Anthony Yoshimura<sup>2</sup>; Nikhil Koratkar<sup>3</sup>; Saroj Nayak<sup>1</sup>; Kisor Sahu<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bhubaneswar; <sup>2</sup>Livermore National Laboratory; <sup>3</sup>Rensselaer Polytechnic Institute

**Predicting Glass Behaviour from Optical Microscopy Images Using Interpretable Machine Learning:** *Ankur Agrawal*<sup>1</sup>; *Mohd Zakri*<sup>1</sup>; Ravinder Bhattoo<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi

## ARTIFICIAL INTELLIGENCE

### Accelerating Materials Science with Big Data and Machine Learning — On-Demand Poster Presentations

**Program Organizers:** Huan Tran, Georgia Institute of Technology; Muratahan Aykol, Toyota Research Institute

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Developing Physics-based Descriptors for Property Prediction in Oxide Glasses:** *Suresh Bishnoi*<sup>1</sup>; Ravinder Ravinder<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology, Delhi

**Machine Learning to Predict Mechanical Properties of Steel Alloys Based on Chemical Composition and Heat Treatment Process:** *Yutao Wang*<sup>1</sup>; <sup>1</sup>WPI

**Topology Optimization for Two-phase Composites Using Active Learning Based Gaussian Process Regression:** *Tanu Pittie*<sup>1</sup>; Suresh Bishnoi<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (IIT), Delhi

## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — AM Modeling - On-Demand Oral Presentations

**Sponsored by:** TMS Computational Materials Science and Engineering Committee

**Program Organizers:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**Session Chair:** Jing Zhang, Indiana University - Purdue University Indianapolis

**Grain Refinement and Mechanical Properties for AISI304 Stainless Steel Single-tracks by Laser Melting Deposition: Mathematical Modelling versus Experimental Results:** *Muhammad Arif Mahmood*<sup>1</sup>; Andrei C. Popescu<sup>1</sup>; Mihai Oane<sup>1</sup>; Diana Chioibas<sup>1</sup>; Gianina Popescu-Pelin<sup>1</sup>; Carmen Ristoscu<sup>1</sup>; Ion N. Mihailescu<sup>1</sup>; <sup>1</sup>National Institute for Laser, Plasma and Radiation Physics (INFLPR)

**Numerical Simulations of Fracture Tests of Uncharged and Hydrogen-charged Bend Specimens of Additively Manufactured 304 Stainless Steel Using Nodal Release Method and Cohesive Zone Model:** *Shengjia Wu*<sup>1</sup>; Shin-Jang Sung<sup>1</sup>; Jwo Pan<sup>1</sup>; Paul Korinko<sup>2</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>Savannah River National Laboratory

**Ductile Fracture of Ti-6Al-4V Made by Powder Bed Fusion Additive Manufacturing:** *Allison Beese*<sup>1</sup>; Alexander Wilson-Heid<sup>1</sup>; <sup>1</sup>Pennsylvania State University

# Technical Program

**Thermal History of LPBF Components Towards Predicting As-built Material Properties:** Martin Verhulsdonk<sup>1</sup>; Simon Vervoort<sup>1</sup>; *Mustafa Megahed*<sup>2</sup>; <sup>1</sup>Fraunhofer Institute for Laser Technology ILT; <sup>2</sup>ESI Group

**Defect Prediction thru Part-scale Simulation:** *Shawn Hinnebusch*<sup>1</sup>; Florian Dugast<sup>1</sup>; Alaa Olleak<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**Inherent Strain Method for Residual Stress Prediction in Ferritic-austenitic Steel Structure Fabricated by Directed Energy Deposition:** *Zhengdong Shan*<sup>1</sup>; Minh Tien Tran<sup>1</sup>; Huai Wang<sup>2</sup>; Sun-Kwang Hwang<sup>3</sup>; Dong-Kyu Kim<sup>1</sup>; <sup>1</sup>University of Ulsan; <sup>2</sup>Chinese Academy of Sciences; <sup>3</sup>Korea Institute of Industrial Technology

**Deep Learning Prediction of Stress Fields in Additively Manufactured Metals with Intricate Defect Networks:** *Brendan Croom*<sup>1</sup>; Michael Berkson<sup>1</sup>; Bobby Mueller<sup>1</sup>; Michael Presley<sup>1</sup>; Steven Storck<sup>1</sup>; <sup>1</sup>JHU Applied Physics Laboratory

**Process Maps and Models For Highly Filled Polymers In Powder Fused Filament Fabrication (PF3) 3D Printing:** *Kameswara Pavan Ajarapu*<sup>1</sup>; Roshan Mishra<sup>1</sup>; Ji-Hae Kim<sup>1</sup>; Kunal Kate<sup>1</sup>; <sup>1</sup>University of Louisville

**Modeling Collapse Behavior in Large-scale Thermoset Additive Manufacturing:** *Stian Romberg*<sup>1</sup>; Chris Hershey<sup>2</sup>; John Lindahl<sup>2</sup>; Abrian Abir<sup>3</sup>; Michael DeVinney<sup>4</sup>; Chad Duty<sup>1</sup>; Vlastimil Kunc<sup>2</sup>; Brett Compton<sup>3</sup>; <sup>1</sup>University of Tennessee, Knoxville; Oak Ridge National Laboratory; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>University of Tennessee, Knoxville; <sup>4</sup>

**Interfacial Properties in 3D Printed Stainless Steel Coated with Epoxy:** *Xuehui Yang*<sup>1</sup>; Sugrim Sagar<sup>1</sup>; Tejesh Dube<sup>1</sup>; Alan Jones<sup>1</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis

**Mechanical Properties of Ceramic Core with SiO<sub>2</sub>-Na<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub> Ternary Binder System:** *Hyunhee Choi*<sup>1</sup>; Bong-Gu Kim<sup>2</sup>; Eun-Hee Kim<sup>1</sup>; Junseong Kim<sup>2</sup>; Seong-Hwa Jeong<sup>2</sup>; Seung-Cheol Yang<sup>2</sup>; Yeon-Gil Jung<sup>2</sup>; <sup>1</sup>Changwon National University; <sup>2</sup>Department of Materials Convergence and System Engineering of Changwon National University

**Preparation of Ceramic Green Body with Uniform Density through Living Properties of Cycloaliphatic Epoxy Resins in DLP(Digital Light Processing) 3D Printing of Ceramics:** *Hye-Yeong Park*<sup>1</sup>; SeungHwa Jeong<sup>2</sup>; Haeun Kim<sup>2</sup>; DongHyun Kim<sup>2</sup>; Janghyeok Pyeon<sup>2</sup>; SeungCheol Yang<sup>1</sup>; Yeon-Gil Jung<sup>1</sup>; <sup>1</sup>Changwon National University; <sup>2</sup>Department of Materials Convergence and System Engineering of Changwon National University

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## ADDITIVE MANUFACTURING

### Additive Manufacturing Modeling and Simulation: Microstructure, Mechanics, and Process — AM Modeling - On-Demand Poster Presentations

**Sponsored by:** TMS Computational Materials Science and Engineering Committee

**Program Organizers:** Jing Zhang, Indiana University – Purdue University Indianapolis; Brandon McWilliams, US Army Research Laboratory; Li Ma, Johns Hopkins University Applied Physics Laboratory; Yeongil Jung, Changwon National University

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On-Demand Poster Hall | MS&T On Demand

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**Model the Initiation of Hot Cracking during Laser Welding of Al6061:** *Guannan Tang*<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Ceramic-based Materials: Process Development, Materials, Process Optimization and Applications — On-Demand Oral Presentations

**Sponsored by:** ACerS Engineering Ceramics Division, ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Xuan Song, University of Iowa; Lei Chen, University of Michigan-Dearborn; Xiangyang Dong, Missouri University of Science and Technology; Yiquan Wu, Alfred University; Paolo Colombo, University of Padova; Rajendra Bordia, Clemson University; Long-Qing Chen, Pennsylvania State University

Friday AM | October 22, 2021  
On-Demand Room 1 | MS&T On Demand

**Session Chair:** Xuan Song, University of Iowa

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## Invited

**Towards Direct Additive Manufacturing of Ceramics by Selective Laser Flash Sintering:** *Desiderio Kovar*<sup>1</sup>; <sup>1</sup>University of Texas at Austin

**Mesoscale Modeling of Sintering Kinetics in Direct Ink Write Additive Manufacturing:** *Fadi Abdeljawad*<sup>1</sup>; <sup>1</sup>Clemson University

**Structure and High Temperature Mechanics of Binder Jet 3D Printed Ceramic Compacts Treated with Reactive Precursors:** *Lynnora Grant*<sup>1</sup>; C. Higgs III<sup>1</sup>; Zachary Cordero<sup>2</sup>; <sup>1</sup>Rice University; <sup>2</sup>Massachusetts Institute of Technology

**Direct-writing by Micro Cold Spray of Yttria (Y2O3) Films:** *Aidan Moyers*<sup>1</sup>; Michael Becker<sup>1</sup>; Desiderio Kovar<sup>1</sup>; <sup>1</sup>The University of Texas at Austin

**Mechanical Properties and Ionic Conductivity of Li<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub>-P<sub>2</sub>O<sub>5</sub> Prepared Using Laser Powder Bed Fusion:** *Katherine Acord*<sup>1</sup>; Alexander Dupuy<sup>1</sup>; Olivia Donaldson<sup>1</sup>; Xin Wang<sup>1</sup>; Timothy Rupert<sup>1</sup>; James Wu<sup>2</sup>; Qian Chen<sup>3</sup>; Julie Schoenung<sup>1</sup>; <sup>1</sup>University of California, Irvine; <sup>2</sup>NASA Glenn Research Center; <sup>3</sup>Jet Propulsion Laboratory



**Improving Ceramic Additive Manufacturing via Machine Learning-enabled Closed-Loop Control:** Zhaolong Zhang<sup>1</sup>; Richard Sisson<sup>1</sup>; Jianyu Liang<sup>1</sup>; *Zhaotong Yang*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**Binder-free Additive Manufacturing of Ceramics Using Hydrothermal-assisted Jet Fusion:** Fan Fei<sup>1</sup>; Levi Kirby<sup>1</sup>; *Xuan Song*<sup>1</sup>; <sup>1</sup>University of Iowa

**Effect of Particle Morphology and Green Part Density on Microstructure Evolution and Mechanical Properties of Sintered Alumina Fabricated via Ceramic Fused Filament Fabrication (CF3):** Kameswara Pavan Ajjarapu<sup>1</sup>; Kavish Sudan<sup>1</sup>; Kunal Kate<sup>1</sup>; <sup>1</sup>University of Louisville

**3D Printed Ceramic Acoustic Liners for Aircraft Noise Reduction:** David Nevarez-Saenz<sup>1</sup>; Ted Adler<sup>1</sup>; Wei Wei<sup>1</sup>; Bhisham Sharma<sup>1</sup>; <sup>1</sup>Wichita State University

**Micro-cold Spray: Influence of SiC Nanoparticle Impact Angle on Deformation Behavior:** Derek Davies<sup>1</sup>; Michael Gammage<sup>2</sup>; Michael Becker<sup>1</sup>; John Keto<sup>1</sup>; Desiderio Kovar<sup>1</sup>; <sup>1</sup>The University of Texas at Austin; <sup>2</sup>CCDC DEVCOM Army Research Laboratory

#### ADDITIVE MANUFACTURING

**Additive Manufacturing of Ceramic-based Materials: Process Development, Materials, Process Optimization and Applications — On-Demand Poster Presentations**

**Sponsored by:** ACerS Engineering Ceramics Division, ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Xuan Song, University of Iowa; Lei Chen, University of Michigan-Dearborn; Xiangyang Dong, Missouri University of Science and Technology; Yiquan Wu, Alfred University; Paolo Colombo, University of Padova; Rajendra Bordia, Clemson University; Long-Qing Chen, Pennsylvania State University

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Properties of LiNbO<sub>3</sub> Films Deposited by Micro-Cold Spray at Varying Angles of Impact:** Stephen Bierschenk<sup>1</sup>; Michael Becker<sup>1</sup>; Susanne Lee<sup>2</sup>; Desiderio Kovar<sup>1</sup>; <sup>1</sup>The University of Texas at Austin; <sup>2</sup>L3Harris Technologies, Inc.

#### ADDITIVE MANUFACTURING

**Additive Manufacturing of High and Ultra-High Temperature Ceramics and Composites: Processing, Characterization and Testing — On-Demand Oral Presentations**

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Corson Cramer, Oak Ridge National Laboratory; Greg Hilmas, Missouri University of Science and Technology; Lisa Rueschhoff, Air Force Research Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**Additive Manufacturing of Silicon Nitride Using a Slurry Approach:** Beth Armstrong<sup>1</sup>; Corson Cramer<sup>1</sup>; Benjamin Lamm<sup>1</sup>; Trevor Aguirre<sup>1</sup>; David Mitchell<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**Investigation of Oxidation Behavior of ZrB<sub>2</sub>-SiC Composites under Different Partial Pressures of Oxygen:** Rubia Hassan<sup>1</sup>; Rishabh Kundu<sup>2</sup>; Kantesh Blaani<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Kanpur; <sup>2</sup>National Institute of Technology Rourkela

**AM of UHTCs at LLNL:** James Cahill<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

**Additive Manufacturing of Corrosion Resistant UHTC Materials for Chloride Salt-to-sCO<sub>2</sub> Brayton Cycle Heat Exchangers:** James Kelly<sup>1</sup>; Jeffery Haslam<sup>1</sup>; Lauren Finkenauer<sup>1</sup>; Michael Ross<sup>1</sup>; Pratanu Roy<sup>1</sup>; Du Nguyen<sup>1</sup>; Joshua Stolaroff<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

**Additive Manufacturing of High-performance Advanced Ceramics by the Ceramic On-demand Extrusion (CODE) Process:** Ming Leu<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

**Molten Chloride Salt Corrosion Testing of Ultra High Temperature Ceramics for High Temperature Heat Exchangers Fabricated by Additive Manufacturing Methods:** Jeffery Haslam<sup>1</sup>; James Kelly<sup>1</sup>; Joshua Stolaroff<sup>1</sup>; Michael Ross<sup>1</sup>; Stephen Raiman<sup>2</sup>; Bruce Pint<sup>3</sup>; Dino Sulemanovic<sup>3</sup>; <sup>1</sup>LLNL; <sup>2</sup>Texas A&M University; <sup>3</sup>Oak Ridge National Laboratory

**Pathways to Additively Manufacture Ultra-high Temperature Ceramic Composites:** James Kemp<sup>1</sup>; Zlatomir Apostolov<sup>2</sup>; Brett Compton<sup>1</sup>; Lisa Rueschhoff<sup>3</sup>; <sup>1</sup>The University of Tennessee, Knoxville; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>Air Force Research Laboratory

**Deposition of UHTC Coatings on Refractory Substrates by Directed Energy Methods:** Zlatomir Apostolov<sup>1</sup>; Noam Eliaz<sup>2</sup>; Michael Cinibulk<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>Tel Aviv University

**Strategies for Printing Continuous Fibers and Post-processing for Ceramic Matrix Composites (CMCs):** Corson Cramer<sup>1</sup>; Vipin Kumar<sup>1</sup>; Ryan Duncan<sup>1</sup>; David Mitchell<sup>1</sup>; Vlastimil Kunc<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory



# Technical Program

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Equipment, Instrumentation and In-Situ Process Monitoring — On-Demand Oral Presentations

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Joy Gockel, Colorado School of Mines; Sneha Prabha Narra, Carnegie Mellon University

Friday AM | October 22, 2021  
On-Demand Room 1 | MS&T On Demand

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**Defect Recognition and Improvement in Ti-6Al-4V Fabrication by In-situ Monitoring and Feedback System of Directed Energy Deposition LAMDA 200:** *Lingxiao Ouyang*<sup>1</sup>; Kenta Aoyagi<sup>1</sup>; Yuji Imamiya<sup>2</sup>; Akihiko Chiba<sup>1</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>Mitsubishi Heavy Industries Machine Tool Co., Ltd.

**Plenoptic Imaging for In-situ PIV and Melt Pool Monitoring in Laser Directed Energy Deposition:** *James Haley*<sup>1</sup>; Thomas Feldhausen<sup>1</sup>; Vincent Paquit<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**Studying the Effect of Inert Gases on Thermal Behavior in Laser Powder Bed Fusion Using In Situ Monitoring and Similarity Analysis:** *Sujana Chandrasekar*<sup>1</sup>; Fred List<sup>2</sup>; Sabina Kumar<sup>1</sup>; Keith Carver<sup>2</sup>; Jamie Coble<sup>1</sup>; Vincent Paquit<sup>2</sup>; Sudarsanam Babu<sup>1</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Oak Ridge National Laboratory

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## ADDITIVE MANUFACTURING

### Additive Manufacturing of Metals: Microstructure, Properties and Alloy Development — On-Demand Oral Presentations

**Program Organizers:** Prashanth Konda Gokuldoss, Tallinn University of Technology; Juergen Eckert, Erich Schmid Institute of Materials Science; Zhi Wang, South China University of Technology

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On-Demand Room 1 | MS&T On Demand

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**Critical Crystallization Properties of an Industrial-Grade Zr-based Metallic Glass-Forming Alloy Used in Additive Manufacturing Measured with Fast Scanning Calorimetry:** *Danielle Kimmel*<sup>1</sup>; *Juergen Schawe*<sup>1</sup>; <sup>1</sup>Mettler Toledo

**Detection and Classification of Internal Defects from Surface Morphology Data of Additively Manufactured Parts:** *Yunwei Gui*<sup>1</sup>; Kenta Aoyagi<sup>1</sup>; Huakang Bian<sup>1</sup>; Akihiko Chiba<sup>1</sup>; <sup>1</sup>Tohoku University

**Cryogenic Mechanical Properties of CrCoNi Medium Entropy Alloy Produced by Selective Laser Melting with Hot Isostatic Pressing:** *Tri Hoang Nguyen*<sup>1</sup>; Minh Tien Tran<sup>1</sup>; Kyung-Hwan Jung<sup>2</sup>; Ho Won Lee<sup>3</sup>; Sun-Kwang Hwang<sup>2</sup>; Dong-Kyu Kim<sup>1</sup>; <sup>1</sup>University of Ulsan; <sup>2</sup>Korea Institute of Industrial Technology; <sup>3</sup>Korea Institute of Materials Science

**Microstructural and Strength Evolution during Aging of an Additively Manufactured Al-Cu-Mn-Zr Alloy:** *Richard Michi*<sup>1</sup>; Kevin Sisco<sup>2</sup>; Sumit Bahl<sup>1</sup>; Jonathan Poplawsky<sup>1</sup>; Lawrence Allard<sup>1</sup>; Ryan Dehoff<sup>1</sup>; Alex Plotkowski<sup>1</sup>; Amit Shyam<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>University of Tennessee, Knoxville

**Microstructure Optimization and Cracks Reduction in Cobalt Based Superalloys Processed by Directed Energy Deposition:** *Thibaut Froeliger*<sup>1</sup>; Louise Toulbi<sup>1</sup>; Didier Locq<sup>1</sup>; Edouard Chauvet<sup>2</sup>; Arnaud Fernandez<sup>2</sup>; Rémy Dendievel<sup>3</sup>; <sup>1</sup>ONERA; <sup>2</sup>Poly-Shape; <sup>3</sup>Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP

**Effect of Atomizing Gas on the Microstructure and Properties of Additively Manufactured 17-4 Precipitation Hardening Steel:** *Kaushalendra Singh*<sup>1</sup>; George Abbott<sup>1</sup>; Atieh Moridi<sup>1</sup>; <sup>1</sup>Cornell University

**Nonlinear Ultrasonic Methods for Nondestructive Evaluation of Additively Manufactured 316L Stainless Steel:** *Madison Sitkiewicz*<sup>1</sup>; Anna Hayes<sup>1</sup>; SeHyuk Park<sup>1</sup>; Tribikram Kundu<sup>1</sup>; Krishna Muralidharan<sup>1</sup>; <sup>1</sup>University of Arizona

**Functionally Graded Materials Designed by In Situ Site-specific Texture Control during Laser Powder Bed Fusion:** *Karl Söfinowski*<sup>1</sup>; Mallory Wittwer<sup>1</sup>; Matteo Seita<sup>1</sup>; <sup>1</sup>Nanyang Technological University

**Development of Pure Magnesium Stochastic Foams by Additive Manufacturing:** *Bandar AlMangour*<sup>1</sup>; Yu-Jin Hwang<sup>2</sup>; Kyu-Sik Kim<sup>3</sup>; Dariusz Grzesiak<sup>4</sup>; Kee-Ahn Lee<sup>3</sup>; <sup>1</sup>King Fahd University of Petroleum and Minerals; <sup>2</sup>Inha University, Incheon; <sup>3</sup>Inha University, Incheon; <sup>4</sup>West Pomeranian University of Technology

**Tensile Deformation Behavior of Additively Manufactured Co-Cr-Mo Lattice Structures:** *Bandar AlMangour*<sup>1</sup>; So-Yeon Park<sup>2</sup>; Kyu-Sik Kim<sup>2</sup>; Dariusz Grzesiak<sup>3</sup>; Kee-Ahn Lee<sup>2</sup>; <sup>1</sup>King Fahd University of Petroleum and Minerals; <sup>2</sup>Inha University, Incheon; <sup>3</sup>West Pomeranian University of Technology

**Understanding the Microstructure and Magnetic Properties of the L-PBF Nd-Fe-B Permanent Magnetic Material:** *Julan Wu*<sup>1</sup>; <sup>1</sup>University of Nottingham

**Effects of Controlled Porosity on Additively Manufactured Stainless Steel 316L Subject to Dynamic Loading:** *Katie Koube*<sup>1</sup>; Kevin Lamb<sup>2</sup>; Taylor Sloop<sup>1</sup>; Sudarsanam Babu<sup>2</sup>; Naresh Thadhani<sup>1</sup>; Josh Kacher<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>University of Tennessee Knoxville

**An Investigation of Elastic Properties of Coal-derived Graphene-reinforced Aluminum Nanocomposites Using Friction Stir Welding and Molecular Dynamics Simulations:** *Saurav Kar*<sup>1</sup>; Roop Mahajan<sup>1</sup>; <sup>1</sup>Virginia Tech

**Oxide Layer Delamination during Single Cu Microparticle Impacts at High-velocity:** *Ahmed Alade Tiamiyu*<sup>1</sup>; Yuchen Sun<sup>1</sup>; Keith Nelson<sup>1</sup>; Christopher Schuh<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**Influence of Bead's Geometry on the Residual Stresses, Structure and Mechanical Behavior in Wire Arc Additive Manufacturing:** *Ahmed Elsokaty*<sup>1</sup>; Sameha Sadek<sup>1</sup>; Maha Elsaied<sup>1</sup>; Omar Gadalla<sup>1</sup>; Hadeer Achraf<sup>1</sup>; *Hanadi Salem*<sup>1</sup>; <sup>1</sup>American University in Cairo

**The Significant Impact of Grain Refiner on Additively Manufactured TiAl Intermetallic Alloy:** *Danni Huang*<sup>1</sup>; Mingxing Zhang<sup>1</sup>; Ming Yan<sup>2</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>Southern University of Science and Technology

**Physical and Mechanical Properties of Aluminium Bronze - Stainless Steel Binary Alloy after Laser Metal Deposition:** *Konstantin Makarenko<sup>1</sup>; Oleg Dubinin<sup>1</sup>; Igor Shishkovsky<sup>1</sup>; <sup>1</sup>Skolkovo Institute of Science and Technology*

**Effects of Laser Polishing Parameters on Surface Roughness of Additively Manufactured Stainless Steel 316L Parts:** *Daniil Panov<sup>1</sup>; Oleg Oreshkin<sup>2</sup>; Igor Shishkovsky<sup>1</sup>; <sup>1</sup>Skolkovo Institute of Science and Technology; <sup>2</sup>National Research Nuclear University MEPhI*

#### ADDITIVE MANUFACTURING

**Additive Manufacturing of Metals: ICME Gaps: Material Property and Validation Data to Support Certification — On-Demand Oral Presentations**

**Sponsored by:** TMS: Integrated Computational Materials Engineering Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Joshua Fody, NASA Langley Research Center; Edward Glaessgen, NASA Langley Research Center; Christopher Lang, NASA Langley Research Center; Greta Lindwall, KTH Royal Institute of Technology; Michael Sansoucie, NASA Marshall Space Flight Center; Mark Stoudt, National Institute of Standards and Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**Phase Field Informed Monte Carlo Texture Evolution Models for Additive Manufacturing Microstructure Simulation and the Need for Experimental Grain Competition Data:** *Brodan Richter<sup>1</sup>; Joseph Pauza<sup>2</sup>; Anthony Rollett<sup>2</sup>; Edward Glaessgen<sup>1</sup>; <sup>1</sup>NASA Langley Research Center; <sup>2</sup>Carnegie Mellon University*

**CFD Modelling for AM Processes:** *Pareekshith Allu<sup>1</sup>; <sup>1</sup>Flow Science Inc.*

**On Scan Path Knowledge for Model Informed Process Planning and Material Quality Predictions:** *Emil Duong<sup>1</sup>; Lukas Masseling<sup>1</sup>; Ulrich Thombansen<sup>1</sup>; Christian Knaak<sup>1</sup>; Mustafa Megahed<sup>2</sup>; <sup>1</sup>Fraunhofer Institute for Laser Technology ILT; <sup>2</sup>ESI Group*

**Predicting Melt Properties Using Atomistic Simulations with a Highly Accurate Physically Informed Neural Network Interatomic Potential:** *Vesselin Yamakov<sup>1</sup>; Yuri Mishin<sup>2</sup>; Edward Glaessgen<sup>3</sup>; <sup>1</sup>National Institute of Aerospace; <sup>2</sup>George Mason University; <sup>3</sup>NASA Langley Research Center*

**Capturing and Analyzing In-situ Data within the Directed Energy Deposition Process with DEDSmart:** *Michael Juhasz<sup>1</sup>; Melanie Lang<sup>1</sup>; <sup>1</sup>FormAlloy*

#### ADDITIVE MANUFACTURING

**Additive Manufacturing: Advanced Characterization for Industrial Applications — On-Demand Oral Presentations**

**Sponsored by:** TMS Advanced Characterization, Testing, and Simulation Committee, TMS Additive Manufacturing Bridge Committee

**Program Organizers:** Nadia Kouraytem, Utah State University; Fan Zhang, National Institute of Standards and Technology; Lianyi Chen, University of Wisconsin-Madison

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

#### Invited

**Operando Synchrotron X-ray Studies of Metal Additive Manufacturing: From Fundamentals to Industrial Applications:** *Tao Sun<sup>1</sup>; <sup>1</sup>University of Virginia*

**Thermo-mechanical Behavior of AM and Wrought IN718 Under High-strain-rate Tensile Deformation:** *Owen Kingstedt<sup>1</sup>; John Varga<sup>2</sup>; S-Danial Salehi<sup>1</sup>; <sup>1</sup>University of Utah; <sup>2</sup>Sandia National Laboratory*

**Predicting Failure Location in Additively Manufactured Metals Using an Improved Void Descriptor Function:** *Dillon Watring<sup>1</sup>; Jake Benzing<sup>2</sup>; Orion Kafka<sup>2</sup>; Newell Moser<sup>2</sup>; Li-Anne Liew<sup>2</sup>; John Erickson<sup>3</sup>; Nikolas Hrabe<sup>2</sup>; Ashley Spear<sup>1</sup>; <sup>1</sup>University of Utah; <sup>2</sup>National Institute of Standards and Technology; <sup>3</sup>Sandia National Laboratories*

**In-situ Characterization of Pore Formation Dynamics in Pulsed Wave Laser Powder Bed Fusion:** *Seyed Mohammad Hojjatzadeh<sup>1</sup>; Qilin Guo<sup>2</sup>; Niranjana Parab<sup>2</sup>; Minglei Qu<sup>1</sup>; Luis Escano<sup>1</sup>; Kamel Fezzaa<sup>2</sup>; Wes Everhart<sup>3</sup>; Lianyi Chen<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>Argonne National Laboratory; <sup>3</sup>Department of Energy's Kansas City National Security Campus Managed by Honeywell FM&T*

#### ADDITIVE MANUFACTURING

**Additive Manufacturing: Alloy Design to Develop New Feedstock Materials III — On-Demand Oral Presentations**

**Sponsored by:** TMS Alloy Phases Committee

**Program Organizers:** Aurelien Perron, Lawrence Livermore National Laboratory; Joseph McKeown, Lawrence Livermore National Laboratory; Manyalibo Matthews, Lawrence Livermore National Laboratory; Peter Hosemann, University of California, Berkeley; Christian Leinenbach, Empa, Swiss Federal Laboratories for Materials Science and Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**Spherical Micro/Macro Indentation Stress-strain Curves for Additive Manufacturing Materials Design:** *Jordan Weaver<sup>1</sup>; Patxi Fernandez-Zelaia<sup>2</sup>; Houshang Yin<sup>3</sup>; Xiaoyuan Lou<sup>3</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>Auburn University*

# Technical Program

**Development of Al-Ce Alloys for Additive Manufacturing Using the CALPHAD Method:** *Emily Moore*<sup>1</sup>; Zachary Sims<sup>1</sup>; Hunter Henderson<sup>1</sup>; Orlando Rios<sup>2</sup>; Scott McCall<sup>1</sup>; David Weiss<sup>3</sup>; Aurélien Perron<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>UT Knoxville; <sup>3</sup>Eck Industries

**Solidification Cracking in Binary Al-Cu Alloys (1.5, 3.0, 4.5, 6.0, and 10 wt.% Cu) Additively Manufactured by Laser Powder Bed Fusion:** *Keegan Muller*<sup>1</sup>; Thinh Huynh<sup>1</sup>; Holden Hyer<sup>1</sup>; Sharon Park<sup>1</sup>; Le Zhou<sup>2</sup>; Jeongmin Woo<sup>1</sup>; Abhishek Mehta<sup>1</sup>; Brandon McWilliams<sup>3</sup>; Kyu Cho<sup>3</sup>; Yongho Sohn<sup>1</sup>; <sup>1</sup>University of Central Florida; <sup>2</sup>Marquette University; <sup>3</sup>DEVCOM US Army Research Laboratory

**Additive Manufacturing Feasibility Investigation Using Single Track Study for the Fabrication of Borated Austenitic Stainless Steels via Laser Powder Bed Fusion:** *Abhishek Mehta*<sup>1</sup>; Devin Imholte<sup>2</sup>; Nicolas Woolstenhulme<sup>2</sup>; Daniel Wachs<sup>2</sup>; Yongho Sohn<sup>1</sup>; <sup>1</sup>University of Central Florida; <sup>2</sup>Idaho National Laboratory

**Grain Boundary Engineering of 316L Stainless Steel via Laser Powder Bed Fusion:** *Matteo Seita*<sup>1</sup>; Shubo Gao<sup>1</sup>; <sup>1</sup>Nanyang Technological University

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Large-Scale Metal Additive Manufacturing — On-Demand Oral Presentations

**Program Organizers:** Yousub Lee, Oak Ridge National Laboratory; Antonio Ramirez, Ohio State University; Yashwanth Bandari, Meltio Inc.; Duckbong Kim, Tennessee Technological University; Wei Zhang, Ohio State University

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**Moving Heat Source Process Simulation for Wire Arc Additive Manufacturing via a Mesh-free Method and GPU Computing:** *Xavier Jimenez*<sup>1</sup>; Florian Dugast<sup>1</sup>; Alaa Olleak<sup>1</sup>; Albert To<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**A Proposed Sustainable Framework to Assess Wire Arc Additive Manufacturing Efficiency in Processing of Different Mechanical Components:** *Mohamed Fawzy Mohamed*<sup>1</sup>; Ahmed Salem<sup>1</sup>; Ahmed Elskatly<sup>1</sup>; Hanadi Salem<sup>1</sup>; <sup>1</sup>The American University in Cairo

**Thermo-mechanical FEM Modeling and Machine Learning of Distortion on Overhang Structure in Laser Powder Bed Fusion Additive Manufacturing:** *Xuesong Gao*<sup>1</sup>; Tyler High<sup>1</sup>; Jesse Zhu<sup>2</sup>; Wei Zhang<sup>1</sup>; Hyeyun Song<sup>3</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Cornell University; <sup>3</sup>Edison Welding Institute

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Mechanisms and Mitigation of Aqueous Corrosion and High-temperature Oxidation — On-Demand Oral Presentations

**Program Organizers:** Amir Mostafaei, Illinois Institute of Technology; Yashar Behnamian, University of Alberta; Bryan Webler, Carnegie Mellon University

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**High Temperature Oxidation Behavior of Additively Manufactured ZrB<sub>2</sub>-30vol%SiC in CO<sub>2</sub>:** *Marharyta Lakusta*<sup>1</sup>; Nicholas Timme<sup>2</sup>; William Fahrenholtz<sup>2</sup>; Jeremy Watts<sup>2</sup>; Gregory Hilmas<sup>2</sup>; David Lipke<sup>2</sup>; <sup>1</sup>Missouri University of Science and Technology; <sup>2</sup>Missouri University of Science and Technology

**Effect of Post Processing on the Corrosion Behavior of Selective Laser Melted Nickel Based Super Alloy in Acidic Environment:** *Mythreyi O V*<sup>1</sup>; R Jayaganthan<sup>1</sup>; B K Nagesha<sup>2</sup>; <sup>1</sup>IIT Madras; <sup>2</sup>ISRO, GTRE

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## ADDITIVE MANUFACTURING

### Additive Manufacturing: Processing, Microstructure and Material Properties of Titanium-based Materials — On-Demand Oral Presentations

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Ulf Ackelid, Freemelt AB; Ola Harrysson, North Carolina State University; Peeyush Nandwana, Oak Ridge National Laboratory; Rongpei Shi, Lawrence Livermore National Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 1 | MS&T On Demand**

**Laser Additive Manufacturing Under Reactive Atmosphere: An Approach to Fabricate Ultra-high Strength Commercially Pure Titanium Without Sacrificing Ductility:** *Dawei Wang*<sup>1</sup>; Yangping Dong<sup>1</sup>; Ming Yan<sup>1</sup>; <sup>1</sup>Southern University of Science and Technology

**Additive Manufacturing of Shape Memory NiTi Alloys with High Building Rates:** *Jianing Zhu*<sup>1</sup>; Evgenii Borisov<sup>2</sup>; Eduard Farber<sup>2</sup>; Marcel Hermans<sup>1</sup>; Vera Popovich<sup>1</sup>; <sup>1</sup>Delft University of Technology; <sup>2</sup>Peter the Great Saint-Petersburg Polytechnic University

**Influence of Thermal Treatments on the Microstructure and Mechanical Properties of Ti-6Al-4V Built by Electron Beam Melting (EBM):** *K.S.N. Sesha*<sup>1</sup>; Kenta Yamanaka<sup>1</sup>; Kenta Aoyagi<sup>1</sup>; Akihiko Chiba<sup>1</sup>; <sup>1</sup>Institute for Materials Research, Tohoku University

**Effect of Pores Present in Very Low Volume Fraction on Tensile Properties of Additively Manufactured Titanium Alloys:** *Pankaj Kumar*<sup>1</sup>; K.S. Ravi Chandran<sup>2</sup>; <sup>1</sup>University of New Mexico; <sup>2</sup>University of Utah

**Surface Analysis and Microstructure Characterization of Electron Beam Melted (EBM) Ti-6Al-4V:** *Jared Darius*<sup>1</sup>; Daniel Kenney<sup>1</sup>; Marcos Lugo<sup>1</sup>; <sup>1</sup>Liberty University



**Effect of High Oxygen Content on the Tensile and Fatigue Performance of Selectively Laser Melted (SLM) Ti-6Al-4V in the Hot Isostatic Pressed (HIP) Condition:** *Anne Osantowski<sup>1</sup>; Yuwei Zhai<sup>1</sup>; Oscar Quintana<sup>1</sup>; Weidong Tong<sup>1</sup>; <sup>1</sup>Depuy Synthes*

**Microstructural Instability in Additively Manufactured Gamma-TiAl Alloy:** *Johnson Jacob<sup>1</sup>; Darren Fraser<sup>1</sup>; Stefan Gulizia<sup>1</sup>; <sup>1</sup>CSIRO*

## ENERGY

### Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments – On-Demand Oral Presentations

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Friday AM | October 22, 2021**  
**On-Demand Room 6 | MS&T On Demand**

**Session Chair:** Caitlin Taylor, Los Alamos National Laboratory

#### Invited

**Unraveling Solute-solvent Interactions in Molten Salt Environments Using X-ray Absorption Spectroscopy:** *Simerjeet Gill<sup>1</sup>; <sup>1</sup>Brookhaven National Lab*

#### Invited

**Speciation of Metal Ion Solutes in Molten Salt Matrices for Reactor Applications using Advanced Spectroscopy Techniques:** *Ruchi Gakhar<sup>1</sup>; Michael Woods<sup>1</sup>; Simerjeet Gill<sup>2</sup>; Anatoly Frenkel<sup>3</sup>; Mehmet Topsakal<sup>2</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>Brookhaven National Lab; <sup>3</sup>Stonybrook University*

#### Invited

**Utilizing a Dynamic Segmentation Convolutional Neural Network for Microstructure Analysis:** *Stephen Toller<sup>1</sup>; Luke Scime<sup>1</sup>; Kurt Terrani<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

#### Invited

**Successful, Unsuccessful, and Partially-successful Attempts at Understanding Alloy Corrosion in Molten Salts:** *Stephen Raiman<sup>1</sup>; <sup>1</sup>Texas A&M University*

**High Temperature Mechanical Properties of WC/W2C Composites Fabricated by Reactive Sintering of Powders Colloidally Processed:** *Antonio Javier Sanchez-Herencia<sup>1</sup>; Macarena Garcia-Ayala<sup>1</sup>; Sandra Tarancon<sup>2</sup>; Begoña Ferrari<sup>1</sup>; Jose Ygnacio Pastor<sup>2</sup>; <sup>1</sup>Institute for Ceramic and Glass; <sup>2</sup>ETSI Caminos-UPM*

**Radiation Damage Suppression in AISI-316 Steel Nanoparticles: Implications for the Design of Future Nuclear Materials:** *Emily Aradi<sup>1</sup>; Matheus Tunes<sup>2</sup>; Jacob Lewis-Fell<sup>3</sup>; Graeme Greaves<sup>3</sup>; Steven Donnelly<sup>3</sup>; Jonathan Hinks<sup>3</sup>; <sup>1</sup>University of Manchester; <sup>2</sup>Montanuniversitaet Leoben; <sup>3</sup>University of Huddersfield*

**Effects of He on Nanoscale Mechanical Properties of Er:** *Eric Lang<sup>1</sup>; Caitlin Taylor<sup>2</sup>; Riley Parrish<sup>1</sup>; Patrick Price<sup>1</sup>; Raj Tandon<sup>1</sup>; Khalid Hattar<sup>1</sup>; <sup>1</sup>Sandia National Laboratories; <sup>2</sup>Los Alamos National Lab*

**Characterizing the Spatial and Temporal Evolution of Iron Thin Films during Coupled Irradiation and Corrosion:** *Benjamin Derby<sup>1</sup>; Trevor Clark<sup>2</sup>; Junsoo Han<sup>3</sup>; Khalid Hattar<sup>2</sup>; John Scully<sup>3</sup>; Matthew Janish<sup>1</sup>; Cortney Kreller<sup>1</sup>; Nan Li<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Sandia National Laboratory; <sup>3</sup>University of Virginia*

**Effect of Ion Irradiation on the Corrosion of 304SS in PWR Simulated Water Chemistry:** *Fu-Yun Tsai<sup>1</sup>; Ryan Schoell<sup>1</sup>; Khalid Hattar<sup>2</sup>; Djamel Kaoumi<sup>1</sup>; <sup>1</sup>North Carolina State University; <sup>2</sup>Sandia National Laboratories*

**Material Degradation Pathways of UO<sub>2</sub> under Oxygen, Humidity, and Temperature Probed by XAFS:** *Juejing Liu<sup>1</sup>; Aiping Chen<sup>2</sup>; Joanne Stubbs<sup>3</sup>; Peter Eng<sup>3</sup>; Hongwu Xu<sup>2</sup>; Steven Conradson<sup>1</sup>; Xiaofeng Guo<sup>1</sup>; <sup>1</sup>Washington State University; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>University of Chicago*

**Deep Learning Pipeline for Cavity Segmentation in Transmission Electron Microscopy:** *Chun Yin Wong<sup>1</sup>; Xing Wang<sup>2</sup>; Zhe Fan<sup>3</sup>; Karren More<sup>4</sup>; Sergei Kalinin<sup>4</sup>; Maxim Ziatdinov<sup>4</sup>; <sup>1</sup>University of Tennessee, Knoxville; <sup>2</sup>The Pennsylvania State University, Oak Ridge National Laboratory; <sup>3</sup>Lamar University, Oak Ridge National Laboratory; <sup>4</sup>Oak Ridge National Laboratory*

## ENERGY

### Advanced Characterization of Materials for Nuclear, Radiation, and Extreme Environments – On-Demand Poster Presentations

**Sponsored by:** TMS Nuclear Materials Committee

**Program Organizers:** Cody Dennett, Idaho National Laboratory; Samuel Briggs, Oregon State University; Christopher Barr, Naval Nuclear Laboratory; Michael Short, Massachusetts Institute of Technology; Janelle Wharry, Purdue University; Cheng Sun, Idaho National Laboratory; Caitlin Taylor, Los Alamos National Laboratory; Emily Aradi, University of Manchester; Khalid Hattar, Sandia National Laboratories

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Session Chairs:** Emily Aradi, University of Manchester; Cody Dennett, Idaho National Laboratory

**Effect of Dilute Magnetism in a Topological Insulator:** *Firoza Kabir<sup>1</sup>; <sup>1</sup>University of Central Florida*

**Modeling of Graphite Oxidation in Water Vapor Ingress Accidental Conditions for High Temperature Gas-cooled Reactors:** *Yi Je Cho<sup>1</sup>; Kathy Lu<sup>2</sup>; <sup>1</sup>Virginia Tech; <sup>2</sup>Virginia Polytechnic Institute and State University*

**Prediction Thermo-physical Characteristics Nickel-based Superalloys Directional Crystallization:** *Alexander Glotka<sup>1</sup>; Vadim Olshanskii<sup>1</sup>; <sup>1</sup>Zaporizhzhia Polytechnic National University*



# Technical Program

**Tensile Performance of Diffusion Bonded AA6061-AA6061 Cladding-Cladding Interface for Application in U-10Mo Monolithic Fuel Plates:** *Abhishek Mehta*<sup>1</sup>; Jeongmin Woo<sup>1</sup>; Jeffrey Giglio<sup>2</sup>; Jan-Fong Jue<sup>2</sup>; Dennis Keiser<sup>2</sup>; James Cole<sup>2</sup>; Yongho Sohn<sup>1</sup>; <sup>1</sup>University of Central Florida; <sup>2</sup>Idaho National Laboratory

**The Effect of Rotary Swaging on Zirconium Alloys and its Microstructure Property Correlation:** *Gaurav Singh*<sup>1</sup>; Raviraj Verma<sup>1</sup>; K I Vishnu Narayanan<sup>2</sup>; Umesh Kumar Arora<sup>2</sup>; R. Jayaganthan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Madras; <sup>2</sup>NFC Hyderabad

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Coatings for Wear and Corrosion Protection — On-Demand Oral Presentations

**Program Organizers:** Evelina Vogli, Lm Group Holdings Inc.; Virendra Singh, Schlumberger

Friday AM | October 22, 2021  
On-Demand Room 9 | MS&T On Demand

**Tribological Resistance and Anti-corrosive Properties of Cr-based Electrochemical Nano-composite Coatings Reinforced with Yttria Stabilised Zirconia and Carbon Nanotubes:** *Pragya Tripathi*<sup>1</sup>; Prvan Katiyar<sup>1</sup>; Janakarajan Ramkumar<sup>1</sup>; Kantesh Balani<sup>1</sup>; <sup>1</sup>Indian Institute of Technology

**Electroplated Ni-MMC Coatings as a Base Coating to Improve High Temperature Corrosion Caused by Sodiumvanadates:** *Christoph Grimme*<sup>1</sup>; Robin Kupec<sup>1</sup>; Xabier Montero<sup>1</sup>; Mathias Galetz<sup>1</sup>; <sup>1</sup>Dechema-Forschungsinstitut

**Galvanic Corrosion of AZ31B Ultrasonically-welded with Bare and Zn-coated Steels:** *Jiheon Jun*<sup>1</sup>; Jian Chen<sup>1</sup>; Yong Chae Lim<sup>1</sup>; Michael Brady<sup>1</sup>; Donovan Leonard<sup>1</sup>; Zhili Feng<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Coatings for Wear and Corrosion Protection — On-Demand Poster Presentations

**Program Organizers:** Evelina Vogli, Lm Group Holdings Inc.; Virendra Singh, Schlumberger

Friday AM | October 22, 2021  
On-Demand Poster Hall | MS&T On Demand

**Hot Corrosion Behavior of Yb<sub>2</sub>O<sub>3</sub>-Gd<sub>2</sub>O<sub>3</sub>-Y<sub>2</sub>O<sub>3</sub> Co-Stabilized Zirconia in Thermal Barrier Coatings with a Lewis Neutral Layer:** *Junseong Kim*<sup>1</sup>; Dowon Song<sup>2</sup>; Guanlin Lyu<sup>3</sup>; Janghyeok Pyeon<sup>1</sup>; SeungCheol Yang<sup>1</sup>; Yeon-Gil Jung<sup>1</sup>; <sup>1</sup>Department of Materials Convergence and System Engineering of Changwon National University; <sup>2</sup>Hanyang University; <sup>3</sup>Changwon National University

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Advanced Materials for Harsh Environments — On-Demand Oral Presentations

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Navin Manjooran, Solve Technology and Research, Inc.; Gary Pickrell, Virginia Tech

Friday AM | October 22, 2021  
On-Demand Room 9 | MS&T On Demand

**Investigation of Automotive Materials Compatibility for Regenerative Fuels – Oxymethylene Dimethyl Ether (OME):** *Ruediger Reitz*<sup>1</sup>; <sup>1</sup>Technische Universität Darmstadt

**Structural Response of Si (111) and Diamond/Si (111) to 193 nm and 5 ns Laser Pulses:** *Chaoya Han*<sup>1</sup>; <sup>1</sup>University of Delaware

**Influence of the Gas Composition on the Metal Dusting Attack of Oxide Forming Alloys:** *Clara Schlereth*<sup>1</sup>; Anke Ulrich<sup>1</sup>; Mathias Galetz<sup>1</sup>; <sup>1</sup>DECHEMA-Forschungsinstitut

**Microstructure and Mechanical Properties of Friction Stir Welded Haynes 282:** *Mageshwari Komarasamy*<sup>1</sup>; Christopher Smith<sup>1</sup>; Jens Darsell<sup>1</sup>; Woongjo Choi<sup>1</sup>; Saumyadeep Jana<sup>1</sup>; Anand Kulkarni<sup>2</sup>; Kyle Stoodt<sup>2</sup>; Glenn Grant<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Siemens Corporation

**Enhancing the Hardness and Corrosion Resistance of Ni-based Alloys with Thermomechanical Processing:** *Haruka Shima*<sup>1</sup>; Manami Mori<sup>2</sup>; Kenta Yamanaka<sup>1</sup>; Kazuo Yoshida<sup>1</sup>; Akihiko Chiba<sup>1</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>National Institute of Technology, Sendai College

**Robust Heat Resistant Superhydrophobic Coatings Fabricated by Functionalized Nanoparticles:** *Anna Schmidt-Verma*<sup>1</sup>; Thomas Fischer<sup>1</sup>; Sanjay Mathur<sup>1</sup>; <sup>1</sup>Universität zu Köln

**Finite Element Corrosion Model and Experimental Characterization of Austenitic Stainless-Steel Engine Valves Oxidized in CO<sub>2</sub> at 700 °C:** *Iman Abdallah*<sup>1</sup>; Louis Bailly-Salins<sup>1</sup>; Xueyang Wu<sup>2</sup>; Robert Ullberg<sup>2</sup>; Taeho Kim<sup>1</sup>; Mohamed ElBakhshwan<sup>1</sup>; Mark Carroll<sup>3</sup>; John Perepezko<sup>1</sup>; Wen Jiang<sup>4</sup>; Simon Phillpot<sup>2</sup>; Michael Tonks<sup>2</sup>; Adrien Couet<sup>1</sup>; <sup>1</sup>UW-Madison; <sup>2</sup>University of Florida; <sup>3</sup>Tenneco; <sup>4</sup>Idaho National Laboratory (INL)

**Corrosion Behaviors of Carbon Steels and Cr-bearing Steels in Supercritical CO<sub>2</sub>:** *Kaiyang Li*<sup>1</sup>; Yimin Zeng<sup>1</sup>; <sup>1</sup>CanmetMATERIALS, Natural Resources Canada

**Electrical, Microstructural and Thermomechanical Properties of Doped-LaCrO<sub>3</sub> Ceramics for High Temperature Electronics and Sensing Applications:** *Javier Mena*<sup>1</sup>; Edward Sabolsky<sup>1</sup>; Katarzyna Sabolsky<sup>1</sup>; Konstantinos Sierros<sup>1</sup>; Kavin Sivaneri Varadharajan Idhaim<sup>1</sup>; <sup>1</sup>West Virginia University

**Evaluation of High Temperature Planar Passive Wireless Sensor Fabricated by Stereolithography Process:** *Kavin Sivaneri Varadharajan Id*<sup>1</sup>; Matthew Barre<sup>1</sup>; Zachary Lynch<sup>1</sup>; Engin Ciftiyurek<sup>1</sup>; Katarzyna Sabolsky<sup>1</sup>; Edward Sabolsky<sup>1</sup>; Konstantinos Sierros<sup>1</sup>; Daryl Reynolds<sup>1</sup>; <sup>1</sup>West Virginia University

## IRON AND STEEL (FERROUS ALLOYS)

### Advancements in Steel Structural Refinement — On-Demand Oral Presentations

**Sponsored by:** AIST: Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Charles Enloe, CBMM North America; Emmanuel De Moor, Colorado School of Mines; Jianfeng Wang, General Motors Global Research and Development; Jose Rodriguez-Ibabe, CEIT and TECNUN; Steven Jansto, Research and Development Resources

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

**New Modelling Tools for Nb Microalloyed Plate Rolling Design:** Beatriz Pereda<sup>1</sup>; Jose Rodriguez-Ibabe<sup>1</sup>; Marcelo Rebellato<sup>2</sup>; Pello Uranga<sup>1</sup>; <sup>1</sup>CEIT and TECNUN (University of Navarra); <sup>2</sup>RMS

## ELECTRONIC AND MAGNETIC MATERIALS

### Advances in Dielectric Materials and Electronic Devices — On-Demand Poster Session

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Ubic, Boise State University; Matjaz Spreitzer, Jožef Stefan Institute

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Dielectric NDE for On-line Cure Monitoring and Defect Detection in Engineered Composites:** William Flynn<sup>1</sup>; Bryan Gamboa<sup>1</sup>; Sean Garnsey<sup>1</sup>; Ruyan Guo<sup>1</sup>; Amar Bhalla<sup>1</sup>; <sup>1</sup>University of Texas at San Antonio

**Features on the Structural Phase Transition in La-modified AgNbO<sub>3</sub> Lead-free Ceramics:** Karine Felix Santos de Jesus<sup>1</sup>; Atair Carvalho da Silva<sup>1</sup>; Yanela Mendez-González<sup>2</sup>; Ruyan Guo<sup>3</sup>; Amar Bhalla<sup>3</sup>; Jose de los Santos Guerra<sup>2</sup>; <sup>1</sup>Universidade Federal de Uberlandia; <sup>2</sup>Universidad de La Habana; <sup>3</sup>The University of Texas at San Antonio

**Graphs Theory and Electrophysical Parameters Characterization:** Vojislav Mitic<sup>1</sup>; Aleksandar Stajic<sup>2</sup>; Branislav Randjelovic<sup>1</sup>; Srdjan Ribar<sup>3</sup>; Bojana Markovic<sup>3</sup>; Maria Cebela<sup>4</sup>; Ivana Radovic<sup>5</sup>; Hans Fecht<sup>6</sup>; <sup>1</sup>University Nis; <sup>2</sup>University of Belgrade, Center of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia, Belgrade; <sup>3</sup>University of Belgrade; <sup>4</sup>University of Belgrade, 'VINCA' Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade; <sup>5</sup>University of Belgrade; 'VINCA' Institute of Nuclear Sciences – National Institute of the Republic of Serbia, Belgrade; <sup>6</sup>University Ulm, Institute of Functional Nanosystems FNS

**Study and Physical Characterization of Hybrid PVDF/Ceramic Composites:** Evaristo Alexandre Falcão<sup>1</sup>; Atair Carvalho da Silva<sup>2</sup>; Yanela Mendez-González<sup>3</sup>; Ruyan Guo<sup>4</sup>; Amar Bhalla<sup>4</sup>; Jose de los Santos Guerra<sup>2</sup>; <sup>1</sup>Universidade Federal da Grande Dourados; <sup>2</sup>Universidade Federal de Uberlandia; <sup>3</sup>Universidad de La Habana; <sup>4</sup>The University of Texas at San Antonio

**Sensitivity Analysis on the Application of Direct Piezo-electric Effect Using the Finite-element Extended Complex Variable Method:** Carlos Acosta<sup>1</sup>; Jose de los Santos Guerra<sup>2</sup>; Ruyan Guo<sup>3</sup>; Amar Bhalla<sup>3</sup>; <sup>1</sup>Inghieri Solutions LLC; <sup>2</sup>Universidade Federal de Uberlandia; <sup>3</sup>University of Texas at San Antonio

## ELECTRONIC AND MAGNETIC MATERIALS

### Advances in Dielectric Materials and Electronic Devices — On Demand Oral Presentations

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Amar Bhalla, University of Texas; Ruyan Guo, University of Texas at San Antonio; Rick Ubic, Boise State University; Matjaz Spreitzer, Jožef Stefan Institute

**Friday AM | October 22, 2021**  
**On-Demand Room 5 | MS&T On Demand**

**Session Chair:** Matjaz Spreitzer, Jozef Stefan Institute

## Invited

**Neural Networks, Graph Approach and Fractals Application on Electronics Parameters Determination and Prediction in Perovskite Ceramics:** Vojislav Mitic<sup>1</sup>; Ivana Radovic<sup>2</sup>; Branislav Randjelovic<sup>1</sup>; Srdjan Ribar<sup>3</sup>; Cristine Serpa<sup>4</sup>; Ivana Ilic<sup>1</sup>; Aleksandar Stajic<sup>5</sup>; Vesna Paunovic<sup>1</sup>; Branislav Vlahovic<sup>6</sup>; <sup>1</sup>University of Nis; <sup>2</sup>University of Belgrade, 'VINCA' Institute of Nuclear Sciences – National Institute of the Republic of Serbia; <sup>3</sup>University of Belgrade; <sup>4</sup>ISEL – Instituto Superior de Engenharia de Lisboa do Instituto Politécnico de Lisboa; <sup>5</sup>University of Belgrade, Center of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy – National Institute of the Republic of Serbia; <sup>6</sup>North Carolina Central University (NCCU)

**Effect of Fluoride Substitution on the Morphology and Electrical Properties of Dielectric Storage Material:** Narsingh Singh<sup>1</sup>; Laxman Singh<sup>2</sup>; Dinesh Prajapati<sup>2</sup>; Narayan Singh<sup>2</sup>; Fow-Sen Choa<sup>1</sup>; Bradley Arnold<sup>1</sup>; Kamdeo Mandal<sup>2</sup>; Lisa Kelly<sup>1</sup>; Atendra Kumar<sup>2</sup>; <sup>1</sup>University of Maryland Baltimore County; <sup>2</sup>Indian Institute of Technology, BHU

**Electrical and Dielectric Behaviour of Li-substituted Potassium Sodium Niobate System:** Maryam Azadeh<sup>1</sup>; Till Froemling<sup>1</sup>; Ze Xu<sup>2</sup>; Yixuan Liu<sup>2</sup>; Ke Wang<sup>2</sup>; <sup>1</sup>TU Darmstadt; <sup>2</sup>Tsinghua University

**Epitaxial SrTiO<sub>3</sub> Thin Films on Semiconductor Substrates:** Matjaz Spreitzer<sup>1</sup>; <sup>1</sup>Jožef Stefan Institute

**Structure and Domain Morphology of Quenched Na<sub>1/2</sub>Bi<sub>1/2</sub>TiO<sub>3</sub>-BaTiO<sub>3</sub> Piezoceramics:** Andreas Wohninsland<sup>1</sup>; Ann-Katrin Fetzner<sup>1</sup>; Hans-Joachim Kleebe<sup>1</sup>; Lalitha Kodumudi Venkataraman<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt, Germany

**Comparison of Chemical Treatments for the Modification of VHB 4910's Mechanical Properties:** Isaac Liu<sup>1</sup>; Hector Medina<sup>1</sup>; <sup>1</sup>Liberty University

# Technical Program

**Direct-writing of Embedded Flexible Sensors for Strain and Temperature Monitoring for Stretchable Applications:** *Akshay Kakar*<sup>1</sup>; Derrick Banerjee<sup>1</sup>; Edward Sabolsky<sup>1</sup>; Konstantinos Sierros<sup>1</sup>; <sup>1</sup>West Virginia University

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## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Ferrous Metallurgy — On-Demand Oral Presentations

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Emmanuel De Moor, Colorado School of Mines; Kishlay Mishra, Nucor Castrip Arkansas LLC; Lijia Zhao, ArcelorMittal Global R&D

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

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**New Roll Alloys Concepts Using in Finishing Stands of Rebar Rolling:** Babak Nazari<sup>1</sup>; Adel Sheikhsosseini<sup>1</sup>; Hossein Zakerinia<sup>1</sup>; <sup>1</sup>CSMETAL/Chodan Sazan

**Research on the Phosphate Capacity of CaO-FeO-MgO-SiO<sub>2</sub>-MnO-TiO<sub>2</sub>-V<sub>2</sub>O<sub>5</sub>-P<sub>2</sub>O<sub>5</sub> Slags:** *Yun Zhou*<sup>1</sup>; Rong Zhu<sup>1</sup>; Kai Dong<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

**Radiative Properties of Al-Si Coated 22MnB5 Steel:** *Cameron Klassen*<sup>1</sup>; Boxuan Zhao<sup>1</sup>; Kyle Daun<sup>1</sup>; <sup>1</sup>University of Waterloo

**Studying Processing – Microstructure – Mechanical Property Correlation in a Multi-phase Advanced High Strength Steel:** Monowar Hossain<sup>1</sup>; Sanjeev Sharma<sup>2</sup>; Yanwen Wang<sup>2</sup>; Daniel Stephens<sup>2</sup>; *Nilesh Kumar*<sup>1</sup>; <sup>1</sup>University of Alabama, Tuscaloosa; <sup>2</sup>Nucor Steel Decatur, LLC

**Evaluation of Different Austenitization Sub-Models for 22MnB5 Steel Using Bayesian Model Selection Technique:** *Boxuan Zhao*<sup>1</sup>; Constantin Chiriac<sup>2</sup>; Kyle Daun<sup>1</sup>; <sup>1</sup>University of Waterloo; <sup>2</sup>Ford Motor Company

**Effect of CO<sub>2</sub> Injection into Blast Furnace Tuyeres on Smelting Parameters:** *Juanjuan Jiang*<sup>1</sup>; Rong Zhu<sup>1</sup>; Shengtao Qiu<sup>2</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Central Iron and Steel Research Institute

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## IRON AND STEEL (FERROUS ALLOYS)

### Advances in Metallic Coated Advanced Steels — On-Demand Oral Presentations

**Sponsored by:** AIST: Metallurgy Processing Products and Applications Technology Committee, AIST: Galvanizing Technology Committee

**Program Organizers:** Joseph McDermid, McMaster University; Frank Goodwin, ILZRO

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

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**Liquid Metal Embrittlement of 3rd Generation Advanced High Strength Steel Driven by Nano-intermetallic Phase Formation Along Grain Boundaries:** Yuki Ikeda<sup>1</sup>; Anirban Chakraborty<sup>2</sup>; Hassan Ghassemi-Armaki<sup>2</sup>; *Robert Maass*<sup>1</sup>; <sup>1</sup>Federal Institute for Materials Research and Testing (BAM); <sup>2</sup>ArcelorMittal Global Research and Development

**Insight into the Mechanism of Liquid Metal Embrittlement in Resistance Spot Welding of Zn-coated Dual Phase Steel: The Role of Boron and Silicon:** *Elahe Akbari*<sup>1</sup>; Philipp Kürnsteiner<sup>1</sup>; Peter Oberhumer<sup>1</sup>; Günter Hesser<sup>1</sup>; Heiko Groiss<sup>1</sup>; Martin Arndt<sup>2</sup>; Martin Gruber<sup>2</sup>; Robert Sierlinger<sup>2</sup>; <sup>1</sup>Christian Doppler Laboratory for Nanoscale Phase Transformations, Center of Surface and Nanoanalytics, Johannes Kepler University Linz; <sup>2</sup>Voestalpine Stahl GmbH

**Optimal Wavelength Selection for Improved Multi-wavelength Pyrometry of Advanced High Strength Steel:** *Fatima Suleiman*<sup>1</sup>; Kaihsiang Lin<sup>1</sup>; Kyle Daun<sup>1</sup>; <sup>1</sup>University of Waterloo

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## PROCESSING AND MANUFACTURING

### Advances in Surface Engineering — On-Demand Advances in Surface Engineering

**Sponsored by:** TMS Surface Engineering Committee

**Program Organizers:** Rajeswaran Radhakrishnan, Faraday Technology Inc.; Brian Skinn, Faraday Technology, Inc.; Timothy Hall, Faraday Technology Inc.; Michael Roach, University of Mississippi Medical Center; Sandip Harimkar, Oklahoma State University; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University

**Friday AM | October 22, 2021**  
**On-Demand Room 12 | MS&T On Demand**

**Session Chairs:** Holly Garich, Faraday Technology, Inc.; Rajeswaran Radhakrishnan, Faraday Technology, Inc.

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**High Adhesive Joint Durability of Aluminum Alloys with Chemical Free Treatments:** *John Ho*<sup>1</sup>; Alp Manavbasi<sup>1</sup>; <sup>1</sup>Novelis

**Influences of Varied Electro-discharge Machining Operations on Surface Conditions of a Nickel-Base Superalloy:** *Tim Gabb*<sup>1</sup>; T. Smith<sup>1</sup>; J. Telesman<sup>1</sup>; C. Kantzos<sup>1</sup>; R. Rogers<sup>1</sup>; D. Brinkman<sup>2</sup>; T. Ubienski<sup>2</sup>; <sup>1</sup>NASA Glenn Research Center; <sup>2</sup>HX5 Sierra, LLC



**Ionic Polymer-Metal Composite (IPMC) Degradation Study and Solution Considerations for Biomimetic Thin-film Actuator Applications:** *Allison Arnold<sup>1</sup>; Kevin Sivaneri Varadharajan Idhaian<sup>1</sup>; Lisa Hilgar<sup>1</sup>; William Brion<sup>1</sup>; Edward Sabolsky<sup>1</sup>; Ji Su<sup>2</sup>; <sup>1</sup>West Virginia University; <sup>2</sup>NASA Langley Research Center*

**Mechanical Ball Milling of Gas Atomized Ti48Al2Cr2Nb Powder for Preventing Smoking in Electron Beam Additive Manufacturing Process:** *SeungKyun Yim<sup>1</sup>; Huakang Bian<sup>2</sup>; Keiji Yanagihara<sup>2</sup>; Kenta Aoyagi<sup>2</sup>; Akihiko Chiba<sup>2</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>Institute for Materials Research, Tohoku University*

**Surface Evolution and Corrosion Behavior of Cu-doped Carbide-reinforced Martensitic Steels in a Sulfuric Acid:** *Kenta Yamanaka<sup>1</sup>; Manami Mori<sup>2</sup>; Kazuo Yoshida<sup>1</sup>; Akihiko Chiba<sup>1</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>National Institute of Technology, Sendai College*

**Erosion Resistant and Passively Emitting Composite Coatings for Space Charge Mitigation Applications:** *Rajeswaran Radhakrishnan<sup>1</sup>; Danny Liu<sup>1</sup>; Timothy Hall<sup>1</sup>; Maria Inman<sup>1</sup>; Earl Jennings Taylor<sup>1</sup>; Stephen Snyder<sup>1</sup>; Matthew Robertson<sup>2</sup>; Trace Taylor<sup>2</sup>; JR Dennison<sup>2</sup>; <sup>1</sup>Faraday Technology Inc; <sup>2</sup>Utah State University*

## PROCESSING AND MANUFACTURING

### Advances in Surface Engineering — On-Demand Poster Presentations

**Sponsored by:** TMS Surface Engineering Committee

**Program Organizers:** Rajeswaran Radhakrishnan, Faraday Technology Inc; Brian Skinn, Faraday Technology, Inc.; Timothy Hall, Faraday Technology Inc; Michael Roach, University of Mississippi Medical Center; Sandip Harimkar, Oklahoma State University; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Effect of Laser Shock Peening on Residual Stress Distribution of 304 Austenitic Steel:** *Danbi Song<sup>1</sup>; Ryoohan Kim<sup>1</sup>; Jeong Suh<sup>1</sup>; Dongsig Shin<sup>1</sup>; <sup>1</sup>Korea Institute of Machinery and Materials*

## ARTIFICIAL INTELLIGENCE

### AI for Big Data Problems in Advanced Imaging, Materials Modeling and Automated Synthesis — On-Demand Oral Presentations

**Sponsored by:** TMS: Computational Materials Science and Engineering Committee

**Program Organizers:** Mathew Cherukara, Argonne National Lab; Badri Narayanan, University of Louisville; Subramanian Sankaranarayanan, University of Illinois (Chicago)

**Friday AM | October 22, 2021**  
**On-Demand Room 2 | MS&T On Demand**

#### Invited

**Machine Learning for Automated Experiment in Scanning Probe and Electron Microscopy:** *Sergei Kalinin<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

#### Invited

**Deep Learning and Uncertainty Quantification for Automated Experiments:** *Bobby Sumpter<sup>1</sup>; Ayana Ghosh<sup>1</sup>; Maxim Ziatdinov<sup>1</sup>; Sergei Kalinin<sup>1</sup>; Ondrej Dyck<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory*

**Prediction of Dynamic Properties of LiF and FLiBe Molten Salts with DeepPot Network Potentials:** *Alejandro Rodriguez<sup>2</sup>; Hu Ming<sup>1</sup>; <sup>1</sup>University of South Carolina*

**Understanding the Composition-property Relationship of Glasses Using Interpretable Machine Learning:** *Ravinder Bhattoo<sup>1</sup>; Suresh Bishnoi<sup>1</sup>; Mohd Zaki<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi*

## CERAMIC AND GLASS MATERIALS

### Ceramic Matrix Composites — On-Demand Oral Presentations

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Narottam Bansal, NASA Glenn Research Center; Jacques Lamon, CNRS; Sung Choi, Naval Air Systems Command

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

#### Invited

**Subcritical Crack Growth during Static Fatigue of Hi-Nicalon-S SiC Fiber:** *Randall Hay<sup>1</sup>; Marina Ruggles-Wrenn<sup>1</sup>; <sup>1</sup>U.S. Air Force Research Laboratory; <sup>2</sup>Air Force Institute of Technology*

#### Invited

**Static Fatigue of Hi-Nicalon-S Fiber Tows at Elevated Temperature in Air and in Steam:** *Scott Robertson<sup>1</sup>; Marina Ruggles-Wrenn<sup>1</sup>; Randall Hay<sup>2</sup>; Theodore Shillig<sup>1</sup>; Ronald Mitchell<sup>1</sup>; Brian Kroeger<sup>1</sup>; Logan Gumucio<sup>1</sup>; <sup>1</sup>Air Force Institute of Technology; <sup>2</sup>AFRL*



# Technical Program

**Tribological Performance of HfB<sub>2</sub>-ZrB<sub>2</sub> Based Ultra High Temperature Ceramics Consolidated via Spark Plasma Sintering:** *Shruti Dubey<sup>1</sup>; Kantesh Balani<sup>1</sup>; Ambreen Nisar<sup>2</sup>; Shikha Awasthi<sup>3</sup>; <sup>1</sup>Indian Institute of Technology; <sup>2</sup>Florida International University; <sup>3</sup>Indian Institute of Science Bangalore*

**The Effect of Nanosized Additives on the Properties of Silicon Carbide-based Materials:** *Ihor Hnylytsia*

**Developmental Efforts on Alternative Building Material using Kaolin-based Geopolymer from Local Sources in Nigeria:** *Oluwafemi Adelabu<sup>1</sup>; Oluwagbenga Odewole<sup>2</sup>; Augustine Nsah<sup>2</sup>; Tolulope Akinbogun<sup>2</sup>; <sup>1</sup>University of Johannesburg; <sup>2</sup>Federal University of Technology, Akure*

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## CERAMIC AND GLASS MATERIALS

### Ceramics and Glasses Modeling by Simulations and Machine Learning — On-Demand Oral Presentations

**Sponsored by:** ACerS Glass & Optical Materials Division

**Program Organizers:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

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#### Invited

**Looking for Order in Disorder: Topological Data Analysis of Glass Structure:** *Morten Smedskjaer<sup>1</sup>; Søren Sørensen<sup>1</sup>; Christophe Biscio<sup>1</sup>; Lisbeth Fajstrup<sup>1</sup>; Mathieu Bauchy<sup>2</sup>; <sup>1</sup>Aalborg University; <sup>2</sup>University of California, Los Angeles*

#### Invited

**Graph ODE for Learning Dynamic Systems:** *Yizhou Sun<sup>1</sup>; Wei Wang<sup>1</sup>; Zijie Huang<sup>1</sup>; <sup>1</sup>UCLA*

**Machine Learning as a Tool to Accelerate the Design of Nuclear Waste Glasses with Enhanced Sulfur Loadings:** *Taihao Han<sup>1</sup>; Xinyi Xu<sup>2</sup>; Jie Huang<sup>1</sup>; Albert A. Kruger<sup>3</sup>; Aditya Kumar<sup>1</sup>; Ashutosh Goel<sup>2</sup>; <sup>1</sup>Missouri University of Science and Technology; <sup>2</sup>Rutgers, The State University of New Jersey; <sup>3</sup>U.S. Department of Energy, Office of River Protection*

**Decomposing the Strength of Hydrated Cement Compositions by Machine Learning:** *Yu Song<sup>1</sup>; Gaurav Sant<sup>1</sup>; Mathieu Bauchy<sup>1</sup>; <sup>1</sup>University of California, Los Angeles*

**Toward Revealing Full Atomic Picture of Nanoindentation Deformation Mechanisms in Li<sub>2</sub>O-2SiO<sub>2</sub> Glass-ceramics:** *Binghui Deng<sup>1</sup>; <sup>1</sup>Corning Inc*

**Modeling Polaron Hopping in Ternary Spinel Oxides:** *Maytal Caspary Toroker<sup>1</sup>; <sup>1</sup>Technion - Israel Institute of Technology*

**Impact of Irradiation on the Properties of Gel Layer Formed After Aqueous Corrosion of Borosilicate Glasses:** *Amreen Jan<sup>1</sup>; N.M Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi*

**Elucidating Compositional Governance of Optical Properties Oxide Glasses Using Interpretable Machine Learning:** *Mohd Zakri<sup>1</sup>; Vineeth Venugopal<sup>1</sup>; Ravinder Bhattoo<sup>1</sup>; Suresh Bishnoi<sup>1</sup>; Sourabh Kumar Singh<sup>1</sup>; Amarnath R. Allu<sup>2</sup>; Jayadeva<sup>1</sup>; N. M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi; <sup>2</sup>Glass Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata*

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## CERAMIC AND GLASS MATERIALS

### Ceramics and Glasses Modeling by Simulations and Machine Learning — On-Demand Poster Presentations

**Sponsored by:** ACerS Glass & Optical Materials Division

**Program Organizers:** Mathieu Bauchy, University of California, Los Angeles; Peter Kroll, University of Texas at Arlington; N. M. Anoop Krishnan, Indian Institute of Technology Delhi

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

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**Effect of Polydispersity on the Fracture Properties of Calcium-Silicate-Hydrate Gel:** *Ashish Yadav<sup>1</sup>; N.M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (IIT), Delhi*

**Deciphering the Viscosity of Glass Materials with Machine Learning:** *Yu Song<sup>1</sup>; Mathieu Bauchy<sup>1</sup>; <sup>1</sup>University of California, Los Angeles*

**Development of a Transferable Inter-atomic Potential for Boroaluminosilicate Glasses:** *Rajesh Kumar<sup>1</sup>; N M Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Delhi*

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Coatings to Protect Materials from Extreme Environments — On-Demand Coatings for Extreme Environments

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Kang Lee, NASA Glenn Research Center; Yutaka Kagawa, The University of Tokyo; Daniel Mumm, University of California, Irvine; Rodney Trice, Purdue University; Emmanuel Boakye, UES Inc.; Valerie Wiesner, NASA Langley Research Center; Edward Gorzkowski, Naval Research Laboratory; Scooter Johnson, Naval Research Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 9 | MS&T On Demand**

**Session Chair:** Emmanuel Boakye, UES Inc.

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#### Invited

**Modelling Oxygen Permeability through Top Coat and Thermally Grown Oxide in Dense Yb<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> Environmental Barrier Coatings:** *Kuiying Chen<sup>1</sup>; <sup>1</sup>NRC*

**Obtaining Surface Titanium Coatings for Enhance the Material Performance in SHS Conditions:** *Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University*

**Obtaining Surface Coatings Providing Protection Against High Temperatures in the Production of Coke:** *Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; <sup>1</sup>Dneprovsky State Technical University*

**Coatings for Improving the High Temperature Oxidation Resistance of Mo-based Systems:** *Katharina Beck<sup>1</sup>; Frauke Hinrichs<sup>2</sup>; Martin Heilmair<sup>2</sup>; Anke Ulrich<sup>1</sup>; Mathias Galetz<sup>1</sup>; <sup>1</sup>DECHEMA-Forschungsinstitut; <sup>2</sup>Karlsruher Institut für Technologie*

**In-Situ Ceramic Oxide Coating on Stainless Steels for Molten Salt Corrosion Prevention for Concentrated Solar Power Applications:** Animesh Kundu<sup>1</sup>; Sreya Dutta<sup>2</sup>; Chase Clapp<sup>1</sup>; Hannah Clarkson<sup>1</sup>; <sup>1</sup>Lehigh University; <sup>2</sup>Dynalene, Inc

#### MATERIALS-ENVIRONMENT INTERACTIONS

### Coatings to Protect Materials from Extreme Environments — On-Demand Poster Presentations

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Kang Lee, NASA Glenn Research Center; Yutaka Kagawa, The University of Tokyo; Daniel Mumm, University of California, Irvine; Rodney Trice, Purdue University; Emmanuel Boakye, UES Inc.; Valerie Wiesner, NASA Langley Research Center; Edward Gorzkowski, Naval Research Laboratory; Scooter Johnson, Naval Research Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Thermal and Mechanical Properties of  $Y_3(Nb_{1-x}Ta_x)O_7$  as a Material for Thermal Barrier Coating:** Janghyeok Pyeon<sup>1</sup>; Dowon Song<sup>2</sup>; Gualin Lyu<sup>3</sup>; Junseong Kim<sup>3</sup>; Seungcheol Yang<sup>3</sup>; Yeongil Jung<sup>3</sup>; <sup>1</sup>Materials Convergence and System Engineering of Changwon National University; <sup>2</sup>Hangyang University; <sup>3</sup>Changwon National University

**Self-generated Tribo-coatings on Glass from Nano-dispersions in Aqueous Medium:** Sourav Sahoo<sup>1</sup>; Om Khatri<sup>2</sup>; N. M. Anoop Krishnan<sup>1</sup>; Nitya Goswami<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (IIT) Delhi; <sup>2</sup>CSIR-Indian Institute of Petroleum

#### MATERIALS-ENVIRONMENT INTERACTIONS

### Computation Assisted Materials Development for Improved Corrosion Resistance — On-Demand Oral Presentations

**Program Organizers:** Rishi Pillai, Oak Ridge National Laboratory; Laurence Marks, Northwestern University

**Friday AM | October 22, 2021**  
**On-Demand Room 9 | MS&T On Demand**

**Modelling Alkoxide Corrosion Initiation of Pure-aluminum in Ethanol with Integrated Simulation-based Experimental Methods:** Visheet Arya<sup>1</sup>; Rüdiger Reitz<sup>1</sup>; Matthias Oechsner<sup>1</sup>; Eugen Gazenbiller<sup>1</sup>; Daniel Höche<sup>1</sup>; <sup>1</sup>MPA-IfW TU Darmstadt

**Morphological Stability of Electrostrictive Thin Films:** Jin Zhang<sup>1</sup>; Peter Voorhees<sup>1</sup>; <sup>1</sup>Northwestern University

**Modelling Microstructural Evolution of Aluminide Coatings on Ni-based Superalloys:** Wencai Leng<sup>1</sup>; Dmitry Naumenko<sup>1</sup>; Rishi Pillai<sup>2</sup>; <sup>1</sup>Forschungszentrum Jülich GmbH; <sup>2</sup>Oak Ridge National Laboratory

**Modeling of High-temperature Corrosion of Zirconium Alloys Using the eXtended Finite Element Method (X-FEM):** Louis Bailly-Salins<sup>1</sup>; Léo Borrel<sup>1</sup>; Wen Jiang<sup>2</sup>; Benjamin Spencer<sup>2</sup>; Koroush Shirvan<sup>3</sup>; Adrien Couet<sup>1</sup>; <sup>1</sup>University of Wisconsin - Madison; <sup>2</sup>Idaho National Laboratory; <sup>3</sup>Massachusetts Institute of Technology

**First Steps Towards a Coupled Thermodynamic-kinetic Model to Predict Sulfate Deposit Induced Hot Corrosion of Aluminized Ni-based Superalloys:** Yaping Wang<sup>1</sup>; Rishi Pillai<sup>2</sup>; Elena Yazhenskikh<sup>1</sup>; Michael Müller<sup>1</sup>; Dmitry Naumenko<sup>1</sup>; <sup>1</sup>Forschungszentrum Jülich; <sup>2</sup>Oak Ridge National Laboratory

#### MATERIALS-ENVIRONMENT INTERACTIONS

### Computation Assisted Materials Development for Improved Corrosion Resistance — On-Demand Poster Presentations

**Program Organizers:** Rishi Pillai, Oak Ridge National Laboratory; Laurence Marks, Northwestern University

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Predictive Modeling of Microstructure Induced Variations in the Sensitization Response of 5XXX Aluminum Alloys:** Likun Sun<sup>1</sup>; Syeda Noor E Sumaiya<sup>1</sup>; Matthew Steiner<sup>1</sup>; <sup>1</sup>University of Cincinnati

#### NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**Friday AM | October 22, 2021**  
**On-Demand Room 11 | MS&T On Demand**

#### Invited

**Surface-engineered CeO<sub>2</sub> Nanocrystals: Catalysis and Beyond:** Ruigang Wang<sup>1</sup>; <sup>1</sup>The University of Alabama

#### Invited

**2D Material and van der Waal Heterostructure Nanoelectromechanical Systems (NEMS):** Philip Feng<sup>1</sup>; <sup>1</sup>University of Florida

#### Invited

**Effects of Layer Thickness and Constituent Material on the Wear and Corrosion Resistance of Nanostructured Multilayers:** Wenbo Wang<sup>1</sup>; Wenjun Cai<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University

# Technical Program

## Invited

**Nanocrystalline Refractory Ceramic Synthesis Using High Char Polymers:** *Matthew Laskoski<sup>1</sup>; Boris Dyatkin<sup>1</sup>; Tristan Butler<sup>1</sup>; <sup>1</sup>US Naval Research Lab*

## Invited

**Supercrystalline Nanocomposites: Boosting and Controlling the Mechanical Behavior of These New Multifunctional Materials:** *Diletta Giuntini<sup>1</sup>; Buesra Bor<sup>2</sup>; Alexander Plunkett<sup>2</sup>; Berta Domenech<sup>2</sup>; Gerold Schneider<sup>2</sup>; <sup>1</sup>Eindhoven University of Technology; <sup>2</sup>Hamburg University of Technology*

## Invited

**Controlling Synthesis of Nanostructures with Nanoscale Phase Diagrams:** *Ricardo Castro<sup>1</sup>; <sup>1</sup>University of California, Davis*

**Ti3C2 MXene-polyvinyl Alcohol Hybrids for Photothermal Self-healing:** *Yi Je Cho<sup>1</sup>; Kathy Lu<sup>2</sup>; <sup>1</sup>Virginia Tech; <sup>2</sup>Virginia Polytechnic Institute and State University*

**Universal Approach towards Metal Chalcogenide Materials from Molecular Building Blocks:** *Veronika Brune<sup>1</sup>; Sanjay Mathur<sup>1</sup>; <sup>1</sup>University of Cologne*

**Single Acid One-pot Process as an Effective Method for Controlled Generation of Coal-derived Graphene Quantum Dots (GQDs):** *Saurav Kar<sup>1</sup>; Roop Mahajan<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University*

## NANOMATERIALS

### Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials — On-Demand Poster Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Haitao Zhang, University of North Carolina at Charlotte; Gurpreet Singh, Kansas State University; Kathy Lu, Virginia Polytechnic Institute and State University; Edward Gorzkowski, Naval Research Laboratory; Jian Shi, Rensselaer Polytechnic University; Michael Naguib, Tulane University; Sanjay Mathur, University of Cologne

**Friday AM | October 22, 2021**

**On-Demand Poster Hall | MS&T On Demand**

**A Comparative Study of Tantalum Disulfide as Lithium-ion and Potassium-ion Batteries:** *Davi Marcelo Soares<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University*

**Tungsten Ditelluride, A Semimetal Transition Metal Dichalcogenide as Active Material for Monovalent-ion Battery Electrodes:** *Davi Marcelo Soares<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University*

## SPECIAL TOPICS

### Curricular Innovations and Continuous Improvement of Academic Programs (and Satisfying ABET along the Way): The Elizabeth Judson Memorial Symposium — On-Demand Oral Presentations

**Sponsored by:** TMS: Accreditation Committee, TMS: Education Committee

**Program Organizers:** Alison Polasik, Campbell University; Susan Gentry, University of California, Davis; Jeffrey Fergus, Auburn University; Assel Aitkaliyeva, University of Florida; Kester Clarke, Colorado School of Mines; Subhadra Gupta, University of Alabama; Gregg Janowski, University of Alabama at Birmingham; M. Norton, Washington State University

**Friday AM | October 22, 2021**

**On-Demand Room 13 | MS&T On Demand**

**An Innovative and Integrated Approach to Materials Selection and Simulation for Engineering Education:** *Lakshana Mohee<sup>1</sup>; Nicola Stefani<sup>1</sup>; <sup>1</sup>ANSYS Granta*

**Assessment of Ceramic Higher Education Curricula in Nigeria and Prospects for 21st Century Learners:** *Oluwafemi Adelabu<sup>1</sup>; <sup>1</sup>Federal University of Technology, Akure*

**Virtually Teaching Materials Science Topics in 20 Minutes:** *Kaitlin Tyler; Alfred Oti<sup>1</sup>; <sup>1</sup>Ansys*

**Introduction to Materials Science and Engineering: an Online Course from a Student's Perspective:** *Joseph Foster<sup>1</sup>; Subhadra Gupta<sup>1</sup>; <sup>1</sup>University of Alabama*

**Optimum Design of Railcar Truck Stand:** *Balin Shrivastava<sup>1</sup>; Akhil Gone<sup>1</sup>; Krishna Medishetty<sup>1</sup>; Raghu Echempati<sup>1</sup>; <sup>1</sup>Kettering University*

## FUNDAMENTALS AND CHARACTERIZATION

### Deformation-induced Phase Transformations — On-Demand Oral Presentations

**Program Organizers:** Yangyang Zhao, Purdue University; Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Janelle Wharry, Purdue University

**Friday AM | October 22, 2021**

**On-Demand Room 7 | MS&T On Demand**

**Engineering Microstructures for Conventionally and Additively Manufactured Ni-based Superalloys:** *Felix Theska<sup>1</sup>; Nima Haghdadi<sup>1</sup>; Sophie Primig<sup>1</sup>; <sup>1</sup>UNSW Sydney*

**Influence of 3D Microstructure on Deformation-induced Martensitic Transformation Studied by In Situ High-energy Diffraction Microscopy and Crystal Plasticity Modeling:** *Ye Tian<sup>1</sup>; Xiaohui Tu<sup>1</sup>; He Liu<sup>2</sup>; Ming Guan<sup>1</sup>; Peter Kenesei<sup>3</sup>; Jun-Sang Park<sup>3</sup>; Robert Suter<sup>2</sup>; Todd Hufnagel<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>Carnegie Mellon University; <sup>3</sup>Argonne National Laboratory*



## FUNDAMENTALS AND CHARACTERIZATION

### Deformation-induced Phase Transformations — On-Demand Poster Presentations

**Program Organizers:** Yangyang Zhao, Purdue University; Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Janelle Wharry, Purdue University

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Wire Size Effect on the Nucleation of Fatigue Cracks Near Non-metallic Inclusions in Superelastic Nitinol:** *Parisa Shabani Nezhad<sup>1</sup>*; Jacob Rusch<sup>1</sup>; John Moore<sup>1</sup>; Dinc Erdeniz<sup>2</sup>; <sup>1</sup>Marquette University; <sup>2</sup>University of Cincinnati

## PROCESSING AND MANUFACTURING

### Development of Light Weight Alloys and Composites — On-Demand Oral Presentations

**Program Organizers:** Ramasis Goswami, Naval Research Laboratory; Nikhil Gupta, New York University; Tanjore Jayaraman, University of Michigan-Dearborn; Aashish Rohatgi, Pacific Northwest National Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 12 | MS&T On Demand**

#### Invited

**Surge for Design and Development of Low-density High Entropy Alloys and Composites:** Nandini Singh<sup>1</sup>; Yagnesh Shadangi<sup>1</sup>; Vivek Kumar Pandey<sup>1</sup>; Vikas Shivam<sup>1</sup>; *Nilay Mukhopadhyay<sup>1</sup>*; <sup>1</sup>Indian Institute of Technology (BHU) Varanasi

**Grain Boundary Relaxation in Nanocrystalline Aluminum:** *Leslie Mushongera<sup>1</sup>*; Wenye Ye<sup>1</sup>; Jake Hohl<sup>1</sup>; Pradeep Menezes<sup>1</sup>; Mano Misra<sup>1</sup>; <sup>1</sup>University of Nevada Reno

**Effect of Copper Contents on Corrosion of High Performance ACMZ Cast Aluminum Alloys:** *Jiheon Jun<sup>1</sup>*; Amit Shyam<sup>1</sup>; J. Allen Haynes<sup>1</sup>; Yi Feng Su<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

Invited

**Precipitation of Stable Icosahedral Quasicrystalline Phase in Mg-Al-Zn Alloys:** *Alok Singh<sup>1</sup>*; Takanobu Hiroto<sup>1</sup>; Machiko Ode<sup>1</sup>; Karel Tesar<sup>2</sup>; Hidetoshi Somekawa<sup>1</sup>; Toru Hara<sup>1</sup>; <sup>1</sup>National Institute for Materials Science; <sup>2</sup>Czech Technical University in Prague

**Coarsening of Strengthening Phases in Al(Cu) Alloys: Correlated Atomic-Resolution Microscopy and Composition Analysis:** *Ujjval Bansal<sup>1</sup>*; Mahender Singh<sup>1</sup>; Shyam Sinha<sup>1</sup>; Sukla Mondol<sup>2</sup>; Kamanio Chattopadhyay<sup>1</sup>; <sup>1</sup>Indian Institute of Science; <sup>2</sup>NIT Warangal

## IRON AND STEEL (FERROUS ALLOYS)

### Developments in Plate and Line Pipe Steels — On-Demand Oral Presentations

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Daniel Baker, General Motors Corporation; Ashish Singh, Nucor Steel Arkansas; Pello Uranga, CEIT and TECNUN (University of Navarra)

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

**Optimization of Strength and Toughness for Hot-forged Bainitic Medium Carbon Steel using RSM:** *Iman El Mahallawi<sup>1</sup>*; Tamer Mohamed<sup>2</sup>; Abdelwahab Hussein<sup>2</sup>; Ahmed Shash<sup>3</sup>; Taha Mattar<sup>4</sup>; <sup>1</sup>Cairo University/ Adjunct The British University in Egypt; <sup>2</sup>The British University in Egypt; <sup>3</sup>Cairo University/ seconded German University in Cairo; <sup>4</sup>Central Metallurgical Research and Development Institute (CMRDI)

## FUNDAMENTALS AND CHARACTERIZATION

### Emergent Materials under Extremes and Decisive <I>In Situ</I> Characterizations — On-Demand Oral Presentations

**Sponsored by:** ACeRS Basic Science Division

**Program Organizers:** Hongwu Xu, Los Alamos National Laboratory; Xiaofeng Guo, Washington State University; Xujie Lu, Center for High Pressure Science & Technology Advanced Research; Hua Zhou, Argonne National Laboratory; Judith Driscoll, University of Cambridge

**Friday AM | October 22, 2021**  
**On-Demand Room 7 | MS&T On Demand**

**Session Chairs:** Xiaofeng Guo, WSU; Hua Zhou, ANL; Hongwu Xu, LANL

#### Invited

**Nanomechanic Characterizations with Diamond-Anvil Cell Techniques:** *Bin Chen<sup>1</sup>*; Xiaoling Zhou<sup>2</sup>; Jianing Xu<sup>2</sup>; Hongliang Dong<sup>1</sup>; Yanju Wang<sup>1</sup>; Zongqiang Feng<sup>3</sup>; Xiaoxu Huang<sup>3</sup>; <sup>1</sup>Center for High Pressure Science and Technology Advanced Research; <sup>2</sup>Harbin Institute of Technology; <sup>3</sup>Chongqing University

#### Invited

**Nanoparticles Under High Pressure: Assembly and Formation of Active Nanostructures:** *Hongyou Fan<sup>1</sup>*; <sup>1</sup>Sandia National Labs

#### Invited

**Novel Properties in Cuprates Prepared by High Pressure Oxygen Synthesis:** *Steven Conradson<sup>1</sup>*; <sup>1</sup>Jozef Stefan Institute



# Technical Program

## Invited

**Structure and Composition of Novel Nitride Materials Synthesized at Extreme Conditions of High Pressure and High Temperature Determined by Single-crystal X-ray Diffraction and Raman Spectroscopy:** *Alexander Goncharov*<sup>1</sup>; <sup>1</sup>Earth and Planets Laboratory, Carnegie Institution for Science

**New Approach Toward Enhanced Understanding of the Phase Transformation in Anodically Formed Titanium Oxide Nanotubes during Annealing:** *Hammad Malik*<sup>1</sup>; Brian Devener<sup>1</sup>; Jerry Howard<sup>1</sup>; Swomitra Mohanty<sup>1</sup>; Krista Carlson<sup>1</sup>; <sup>1</sup>University of Utah

**Far-From-Equilibrium Processing of Materials under Extreme Conditions:** *Eric O'Quinn*<sup>1</sup>; Alexandre Solomon<sup>1</sup>; Casey Corbridge<sup>1</sup>; Antonio Fuentes<sup>2</sup>; Maik Lang<sup>1</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Cinvestav Unidad Saltillo

**Photoindentation: A New Route to Understanding Dislocation Behavior in Light:** *Atsutomo Nakamura*<sup>1</sup>; *Xufei Fang*<sup>2</sup>; *Ayaka Matsubara*<sup>1</sup>; *Eita Tochigi*<sup>3</sup>; *Yu Oshima*<sup>1</sup>; *Tatsushi Saito*<sup>1</sup>; *Tatsuya Yokoi*<sup>1</sup>; *Yuichi Ikuhara*<sup>3</sup>; *Katsuyuki Matsunaga*<sup>1</sup>; <sup>1</sup>Nagoya University; <sup>2</sup>Technische Universität Darmstadt; <sup>3</sup>The University of Tokyo

**Investigation of Kirkendall Pore Formation and Evolution Using 4D Spatio-Temporal X-ray Tomography and Deep Learning:** *Arun Bhattacharjee*<sup>1</sup>; *Pradyumna Elavarthi*<sup>1</sup>; *Anca Ralescu*<sup>1</sup>; *Ashley Paz y Puente*<sup>1</sup>; <sup>1</sup>University of Cincinnati

## ENERGY

### Energy Materials for Sustainable Development — On Demand Energy Harvesting

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 6 | MS&T On Demand**

## Invited

**Controlling Conductivity in Ferroelectric Oxides at the Nanoscale:** *Dennis Meier*<sup>1</sup>; <sup>1</sup>Norwegian University of Science and Technology, NTNU

## Invited

**Domain-wall Contribution to Weak-field Properties of Lead-based Relaxor Ferroelectrics:** *Tadej Rojac*<sup>1</sup>; *Mirela Dragomir*<sup>1</sup>; *Mojca Otonicar*<sup>1</sup>; <sup>1</sup>Jozef Stefan Institute

## Invited

**Multifunctional Complex Oxide Heterostructures:** *Nini Pryds*<sup>1</sup>; <sup>1</sup>Technical University of Denmark

## Invited

**Structure-Photophysics-Function Relationship of Perovskite Solar Cells:** *He Wang*<sup>1</sup>; <sup>1</sup>University of Miami

## Invited

**Glasses as Energy Materials for a Sustainable Development:** *Monica Ferraris*<sup>1</sup>; *Milena Salvo*<sup>1</sup>; *Federico Smeacetto*<sup>1</sup>; <sup>1</sup>Politecnico di Torino - Italy

## Invited

**Strategies for Enhancement of Energy Storage in Pb-free Ferroic Ceramics for Sustainable Development:** *Ge Wang*<sup>1</sup>; *Zhilun Lu*<sup>1</sup>; *Dawei Wang*<sup>2</sup>; *Antonio Feteira*<sup>3</sup>; *Ian Reaney*<sup>1</sup>; <sup>1</sup>University of Sheffield; <sup>2</sup>Shenzhen Institutes of Advanced Technology; <sup>3</sup>Sheffield Hallam University

## Invited

**Proton Transport in the Ba<sub>0.8</sub>Ca<sub>0.2</sub>NdInO<sub>4</sub> Mixed Oxide Ion Conductor:** *Stephen Skinner*<sup>1</sup>; *Yu Zhou*<sup>1</sup>; <sup>1</sup>Imperial College London

## Invited

**Opto-electric, Opto-mechanical and Opto-thermo-electric Control of Ferroelectric Domains for Multi-source Energy Harvesting and Sensing:** *Yang Bai*<sup>1</sup>; <sup>1</sup>University of Oulu

## Invited

**Processing of Transparent and Luminescent Alumina Polycrystalline Ceramics Doped with Various Rare Earth Elements and Transition Metals:** *Karel Maca*<sup>1</sup>; *Katarina Drdlikova*<sup>1</sup>; *Daniel Drdlik*<sup>1</sup>; *Robert Klement*<sup>2</sup>; *Dusan Galusek*<sup>2</sup>; <sup>1</sup>CEITEC VUT; <sup>2</sup>TnUAD

## Invited

**Charge Extraction by Linearly Increasing Voltage (CELIV): From One-data Point Measurement to Mobility Mapping in Solar Energy Materials:** *Giovanni Fanchini*<sup>1</sup>; *Noah Stocck*<sup>1</sup>; *Miguel Young*<sup>1</sup>; *Tianhao Ouyang*<sup>1</sup>; *Reg Bauld*<sup>1</sup>; <sup>1</sup>University of Western Ontario

**Experimental and Computational Investigations of the Multiple Impurities Effect on the SOFC Cathode Materials:** *Rui Wang*<sup>1</sup>; *Lucas Parent*<sup>1</sup>; *Yu Zhong*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**The Electrical Conductivity and Defect Chemistry of Co, Sc-doped BaZrO<sub>3</sub>:** *Hiroki Uehara*<sup>1</sup>; *Akihiro Ishii*<sup>1</sup>; *Itaru Oikawa*<sup>1</sup>; *Hitoshi Takamura*<sup>1</sup>; <sup>1</sup>Tohoku University

**Enhanced Conductivity Aluminum Composites for Electric Grid Applications:** *Aditya Nittala*<sup>1</sup>; *Lloyd Furuta*<sup>2</sup>; *Kashi Subedi*<sup>2</sup>; *Xiao Li*<sup>1</sup>; *WoongJo Choi*<sup>1</sup>; *David Drabold*<sup>2</sup>; *Alex Poznak*<sup>3</sup>; *Frank Kraft*<sup>2</sup>; *Keerti Kappagantula*<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Ohio University; <sup>3</sup>Hydro Innovation & Technology

## ENERGY

### Energy Materials for Sustainable Development — On Demand Storage and Conversion

**Sponsored by:** ACerS Energy Materials and Systems Division

**Program Organizers:** Armin Feldhoff, Leibniz University Hannover; Kyle Brinkman, Clemson University; Krista Carlson, University of Utah; Eva Hemmer, University of Ottawa; Nikola Kanas, Institute Biosense, University of Novi Sad; Kjell Wiik, Norwegian University of Science and Technology; Lei Zuo, Virginia Tech; Stephanie Lee, Stevens Institute of Technology; Muhammad Hajj, Stevens Institute of Technology; Mohammad Haik, Stevens Institute of Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 6 | MS&T On Demand**

#### Keynote

**Lessons Learned from Materials Enriching Sustainable Energy Storage Solutions:** Ekaterina Pomerantseva<sup>1</sup>; <sup>1</sup>Drexel University

#### Invited

**Advancing Lithium Batteries: An Interdisciplinary Approach:** Nils Peter Wagner<sup>1</sup>; <sup>1</sup>SINTEF

#### Invited

**Solid State Batteries – from Interfaces to High Energy Density:** Jihui Yang<sup>1</sup>; <sup>1</sup>University of Washington

#### Invited

**Electronic Doping of Semiconductor Thermoelectric Nanostructures with Isoelectronic Dopants:** Ayaskanta Sahu<sup>1</sup>; <sup>1</sup>New York University  
 Invited

**Complex Phase Transformations Observed in Na Storage Materials:** Jae Chul Kim<sup>1</sup>; <sup>1</sup>Stevens Institute of Technology

#### Invited

**Half-Heusler Alloys: Promising Materials For Mid-To-High Temperature Thermoelectric Conversion:** Joseph Poon<sup>1</sup>; Mousumi Mitra<sup>1</sup>; Peter Thomas<sup>2</sup>; Kai Yang<sup>2</sup>; <sup>1</sup>University of Virginia; <sup>2</sup>Novus Energy Technologies

#### Invited

**Recovery of Lithium from Geothermal Brines and Minerals:** Mariappan Paranthaman<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

#### Invited

**Recent Advances and Material Challenges in Up-scaling SOEC:** Peter Hendriksen<sup>1</sup>; <sup>1</sup>Technical University of Denmark

#### Invited

**Multifunctional Materials for Solar Technologies:** Federico Rosei<sup>1</sup>; <sup>1</sup>INRS Centre for Energy, Materials and Telecommunications

**Synthesis and Performance Evaluation of Nano TiO<sub>2</sub> (Anatase) Dispersed on Ti<sub>3</sub>C<sub>2</sub>-Mxene as High-performance Anode for Lithium-ion Batteries:** Hanan Tariq<sup>1</sup>; Abdul Shakoor<sup>1</sup>; Jeffin Abraham<sup>1</sup>; Siham Alqaradawi<sup>1</sup>; Ramzan Kahraman<sup>1</sup>; <sup>1</sup>Qatar University

**Fabrication of Microstructurally Engineered Composite Electrodes for SOFC Applications through Additive Manufacturing:** Edward Sabolsky<sup>1</sup>; Joshua Tenney<sup>1</sup>; Gunes Yakaboylu<sup>2</sup>; Jordan Conte<sup>2</sup>; Michael Jones<sup>2</sup>; Irene Fontana<sup>3</sup>; Katarzyna Sabolsky<sup>2</sup>; Harry Abernathy<sup>4</sup>; Gregory Hackett<sup>5</sup>; <sup>1</sup>US Department of Energy- National Energy Technology Laboratory; West Virginia University; <sup>2</sup>West Virginia University; <sup>3</sup>University of Genoa; <sup>4</sup>US Department of Energy- National Energy Technology Laboratory; NETL Support Contractor; <sup>5</sup>US Department of Energy- National Energy Technology Laboratory

**Dense NASICON-type LAGP Ceramics with 2D MoS<sub>2</sub> Interlayer for All-solid-state Lithium Metal Batteries:** Seung Jin Baek<sup>1</sup>; Eunho Cha<sup>1</sup>; Dong Gyu Kim<sup>1</sup>; Do-Kyung Kim<sup>1</sup>; <sup>1</sup>Korea Advanced Institute of Science & Technology

**Au NPs-decorated CeO<sub>2</sub>-TiO<sub>2</sub> for Efficient Photoassisted CO Preferential Oxidation:** Elisa Moretti<sup>1</sup>; Mojtaba Gilzad Kohan<sup>2</sup>; Antonia Infantes Molina<sup>3</sup>; Alberto Vomiero<sup>2</sup>; <sup>1</sup>Ca' Foscari University of Venice; <sup>2</sup>Lulea University of Technology; <sup>3</sup>University of Málaga

**Nano-Catalyst Enhanced Solid Oxide Fuel Cell Anodes for Increased Stability within Hydrocarbon Containing Fuels:** Saad Waseem<sup>1</sup>; Edward Sabolsky<sup>1</sup>; Katarzyna Sabolsky<sup>1</sup>; Richard Hart<sup>2</sup>; Seunghyuck Hong<sup>2</sup>; <sup>1</sup>West Virginia University; <sup>2</sup>GE Research

**A Novel Bi-functional Oxygen Catalyst, NBRO, for Rechargeable Air Battery: Preparation, Characterization, and Catalytic Activity:** Hayato Suzuki<sup>1</sup>; Kentaro Kozasa<sup>1</sup>; Masatsugu Morimitsu<sup>1</sup>; <sup>1</sup>Doshisha University

**Tuning the Thermoelectric Performance of CaMnO<sub>3</sub>-based Ceramics by Controlled Exsolution and Micro-structuring:** Nikola Kanas<sup>1</sup>; Benjamin Williamson<sup>2</sup>; Richard Hinterding<sup>3</sup>; Mari-Ann Einarsrud<sup>2</sup>; Sverre Selbach<sup>2</sup>; Armin Feldhoff<sup>3</sup>; Kjell Wiik<sup>2</sup>; <sup>1</sup>BioSense Institute; <sup>2</sup>NTNU; <sup>3</sup>Leibniz University

**Effects of Processing Conditions on Hybrid Organic-Inorganic Solid Electrolytes:** Vazrik Keshishian<sup>1</sup>; John Kieffer<sup>1</sup>; <sup>1</sup>Vazrik Keshishian

**In-situ Precipitation Processing of High-ionic Conductivity LATP/PEO Solid Electrolyte for Lithium-ion Batteries:** Guangyu Wang<sup>1</sup>; John Kieffer<sup>1</sup>; <sup>1</sup>University of Michigan

**Corrosion Assessment of Duplex Stainless Steels as Candidate Constructional Materials for Pyrolysis Oils Storage and Transportation:** Yimin Zeng<sup>1</sup>; Xue Han<sup>1</sup>; <sup>1</sup>CanmetMATERIALS/Natural Resources Canada

**Transition-metal-mediated Thermal Stability of Spinel Cathode in Li-ion Battery by In Situ Neutron Scattering:** Yan Chen<sup>1</sup>; Ke An<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

# Technical Program

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## CERAMIC AND GLASS MATERIALS

### Engineering Ceramics: Microstructure-Property-Performance Relations and Applications — On-Demand Mechanical Properties of Engineering Ceramics/Applications

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Young-Wook Kim, University of Seoul; Hua-Tay Lin, Guangdong University of Technology; Junichi Tatami, Yokohama National University

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

**Session Chairs:** Junichi Tatami, Yokohama National University; Eita Tochigi, University of Tokyo

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#### Invited

**In Situ and Atomic-scale Investigations of Mechanical Responses in Oxide Crystals:** Eita Tochigi<sup>1</sup>; <sup>1</sup>The University of Tokyo

#### Invited

**Triboluminescence of AlN:Mn and CaAlSiN<sub>3</sub>:Eu Ceramics:** Junichi Tatami<sup>1</sup>; Kentaro Iwai<sup>2</sup>; Motoyuki Iijima<sup>3</sup>; <sup>1</sup>Yokohama National University

**Strengthening and Toughening of Titanium Boride (TiB) Ceramic Material by Metallurgical Control of the Composition of Metallic Phase:** Jun Du<sup>1</sup>; K. S. Ravi Chandran<sup>1</sup>; <sup>1</sup>University of Utah

**Nonlinear Continuum Damage Model for Unidirectional Laminate Based Ceramic Matrix Composites:** Craig Przybyla<sup>1</sup>; Jean-François Maire<sup>2</sup>; Emmanuel Baranger<sup>3</sup>; Frédéric Laurin<sup>2</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>Office National d'Etudes et de Recherches Aéronautiques (ONERA); <sup>3</sup>ENS Paris-Saclay

**Mechanical Properties of Nanocrystalline Ceramics:** Heonjune Ryou<sup>1</sup>; Kevin Anderson<sup>1</sup>; John Drazin<sup>2</sup>; Edward Gorzkowski<sup>1</sup>; Boris Feygelson<sup>1</sup>; James Wollmershauser<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory; <sup>2</sup>Washington State University

**TiB<sub>2</sub>-TiC Based Materials with Fine Microstructure and Improved Mechanical Properties:** Zhezhen Fu<sup>1</sup>; <sup>1</sup>University of Wisconsin Platteville

**Atomistic Modelling of Dynamic Failure in Boron Carbide: Multi-scale Modeling for Materials Design:** Junhao Chang<sup>1</sup>; Benhour Amirian<sup>1</sup>; Matthew Guziewski<sup>2</sup>; James Hogan<sup>1</sup>; <sup>1</sup>University of Alberta; <sup>2</sup>Army Research Laboratory

**Characterization of Clay Ceramics from Areas Near to the Thar Desert, India: Towards Water Filtration Application:** Sunil Duhan<sup>1</sup>; Meraj Warsi<sup>1</sup>; Himanchal Bharadwaj<sup>1</sup>; Pankaj Jakhar<sup>1</sup>; Amrita Nigohkar<sup>1</sup>; Vinayak Shedekar<sup>2</sup>; Anand Plappally<sup>1</sup>; <sup>1</sup>IITJ; <sup>2</sup>The Ohio State University

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## CERAMIC AND GLASS MATERIALS

### Engineering Ceramics: Microstructure-Property-Performance Relations and Applications — On-Demand Poster Presentations

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Young-Wook Kim, University of Seoul; Hua-Tay Lin, Guangdong University of Technology; Junichi Tatami, Yokohama National University

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

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**Discrete Element Modeling of Machining Process for Thermal Barrier Coating:** Jian Zhang<sup>1</sup>; Dan Koo<sup>1</sup>; Hye-Yeong Park<sup>2</sup>; Yeon-Gil Jung<sup>2</sup>; Jing Zhang<sup>1</sup>; <sup>1</sup>Indiana University – Purdue University Indianapolis; <sup>2</sup>Changwon National University

**Engineering Mineral Porosity as a Method for Studying Weathering Rates in Water-rock Systems:** William Taylor<sup>1</sup>; Brian Gorman<sup>1</sup>; Alexis Navarre-Sitchler<sup>1</sup>; <sup>1</sup>Colorado School of Mines

**Low Temperature Pressureless Sintering of Silicon Carbide Ceramics with Aluminum Nitride-Yttria-Ceria-Magnesia:** Eun Seo Kang<sup>1</sup>; Young-Wook Kim<sup>1</sup>; <sup>1</sup>The University of Seoul

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## CERAMIC AND GLASS MATERIALS

### Engineering Ceramics: Microstructure-Property-Performance Relations and Applications — On-Demand Processing-Property Relations

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Young-Wook Kim, University of Seoul; Hua-Tay Lin, Guangdong University of Technology; Junichi Tatami, Yokohama National University

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

**Session Chairs:** Tohru Suzuki, National Institute for Materials Science; Csaba Balazsi, Hungarian Academy of Sciences

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#### Invited

**Investigation and Fabrication of High Thermal Conductivity Silicon Nitride Ceramics:** Hyun Min Lee<sup>1</sup>; Jung Hoon Kong<sup>2</sup>; Do-Kyung Kim<sup>2</sup>; <sup>1</sup>Samsung Electromechanics; <sup>2</sup>Korea Advanced Institute of Science & Technology

#### Invited

**Nanocarbon Added Silicon Nitrides:** Csaba Balazsi<sup>1</sup>; Katalin Balazsi<sup>1</sup>; <sup>1</sup>Centre for Energy Research, Eotvos Lorand Research Network, Hungary

#### Invited

**Fabrication of Transparent Polycrystalline Ceramics by Colloidal Processing and SPS:** Tohru Suzuki<sup>1</sup>; <sup>1</sup>National Institute for Materials Science

**Mechanical, Thermal, and Electrical Properties of Pressureless Sintered SiC Ceramics with BN and C Additives:** *Young-Wook Kim<sup>1</sup>; Rohit Malik<sup>1</sup>; <sup>1</sup>University of Seoul*

**Relationship between the Microstructure and the Mechanical Properties of the MWCNTs Reinforced Potassium-based Metakaolin Alkali Activated Materials:** *Jiaxin Chen<sup>1</sup>; Ange-Therese Akono<sup>1</sup>; <sup>1</sup>Northwestern University*

**Control of Thermal, Electrical, and Mechanical Properties of Porous SiC Ceramics via Doping:** *Shynar Kultayeva<sup>1</sup>; Young-Wook Kim<sup>1</sup>; In-Hyuck Song<sup>2</sup>; <sup>1</sup>University of Seoul; <sup>2</sup>Korea Institute of Materials Science*

## IRON AND STEEL (FERROUS ALLOYS)

### Fracture of Steels: New Approaches to Modeling and Experimental Characterization — On-Demand Oral Presentations

**Sponsored by:** TMS Steels Committee

**Program Organizers:** Louis Hector, General Motors Global Technical Center; Ana Luiza Araujo, AK Steel Research & Innovation; Matthias Militzer, University of British Columbia; Amy Clarke, Colorado School of Mines

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

#### Keynote

**Predicting the Influence of Microstructure on the Strength and Fracture Resistance of Advanced High Strength Steels:** *Allan Bower<sup>1</sup>; <sup>1</sup>Brown University*

## ELECTRONIC AND MAGNETIC MATERIALS

### Functional Defects in Electroceramic Materials — On-Demand Oral Presentations

**Sponsored by:** ACerS Electronics Division

**Program Organizers:** Hui Xiong, Boise State University; Hua Zhou, Argonne National Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 5 | MS&T On Demand**

#### Invited

**Dislocation-based Nanomechanics in Functional Oxides: A Case Study on SrTiO<sub>3</sub>:** *Xufei Fang<sup>1</sup>; Kuan Ding<sup>1</sup>; Stephan Janocha<sup>1</sup>; Christian Minnert<sup>1</sup>; Till Frömling<sup>1</sup>; Karsten Durst<sup>1</sup>; Atsutomo Nakamura<sup>2</sup>; Jürgen Rödel<sup>1</sup>; <sup>1</sup>Technische Universität Darmstadt; <sup>2</sup>Nagoya University*

#### Invited

**Leveraging Structure and Energetics to Enhance Electrochemical Kinetics in Batteries:** *Kai He<sup>1</sup>; <sup>1</sup>Clemson University*

#### Invited

**Modeling the Electrical Double Layer at Solid-state Electrochemical Interfaces:** *Yue Qi<sup>1</sup>; Michael Swift<sup>2</sup>; James Swift<sup>3</sup>; <sup>1</sup>Brown University; <sup>2</sup>Michigan State University; <sup>3</sup>Northern Arizona University*

#### Invited

**Defect-promoted Sulfur Cathode for Highly Stable Sodium-sulfur Batteries:** *Weiyang Li<sup>1</sup>; <sup>1</sup>Dartmouth College*

#### Invited

**Irradiation-enhanced Electrochemical Performance of TiO<sub>2</sub> Anode Material:** *Janelle Wharry<sup>1</sup>; Chao Yang<sup>1</sup>; Tristan Olsen<sup>2</sup>; Hui (Claire) Xiong<sup>2</sup>; Kassiopeia Smith<sup>3</sup>; Yongqiang Wang<sup>4</sup>; Khalid Hattar<sup>5</sup>; Yaqiao Wu<sup>2</sup>; Dmitri Tenne<sup>2</sup>; Sheng Cheng<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Boise State University; <sup>3</sup>National Institute of Standards and Technology; <sup>4</sup>Los Alamos National Laboratory; <sup>5</sup>Sandia National Laboratories*

**Dislocations as "Self-dopants" in Functional Oxides, Exemplified for TiO<sub>2</sub>:** *Qaisar Muhammad<sup>1</sup>; Lukas Porz<sup>1</sup>; Atsutomo Nakamura<sup>2</sup>; Katsuyuki Matsunaga<sup>2</sup>; Marcus Rohnke<sup>3</sup>; Jürgen Janek<sup>3</sup>; Till Frömling<sup>1</sup>; Jürgen Rödel<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt; <sup>2</sup>Nagoya University; <sup>3</sup>Justus Liebig University*

**Ceramics Are Brittle. Can Dislocations Change That?:** *Lukas Porz<sup>1</sup>; Arne Klomp<sup>1</sup>; Xufei Fang<sup>1</sup>; Ning Li<sup>2</sup>; Can Yildirim<sup>3</sup>; Carsten Detlefs<sup>3</sup>; Enrico Bruder<sup>1</sup>; Marion Höfling<sup>1</sup>; Wolfgang Rheinheimer<sup>4</sup>; Eric Patterson<sup>5</sup>; Peng Gao<sup>2</sup>; Karsten Durst<sup>1</sup>; Atsutomo Nakamura<sup>6</sup>; Karsten Albe<sup>1</sup>; Hugh Simons<sup>7</sup>; Jürgen Rödel<sup>1</sup>; <sup>1</sup>Technical University of Darmstadt; <sup>2</sup>Peking University; <sup>3</sup>European Synchrotron Radiation Facility; <sup>4</sup>Forschungszentrum Jülich; <sup>5</sup>US Naval Research Laboratory; <sup>6</sup>Osaka University; <sup>7</sup>Technical University of Denmark*

## CERAMIC AND GLASS MATERIALS

### Glasses and Optical Materials: Current Issues and Functional Applications — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Delia Brauer, Otto Schott Institute of Materials Research

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

#### Invited

**Fracture Toughness of Zeolitic Imidazolate Framework Glasses:** *Morten Smedskjaer<sup>1</sup>; Theany To<sup>1</sup>; Søren Sørensen<sup>1</sup>; Tao Du<sup>1</sup>; Yuanzheng Yue<sup>1</sup>; Mathieu Bauchy<sup>2</sup>; <sup>1</sup>Aalborg University; <sup>2</sup>University of California, Los Angeles*

**Viscoelastic Relaxation in Silica via Reactive Molecular Dynamic Simulations:** *Jessica Rimsza<sup>1</sup>; Scott Grutzik<sup>1</sup>; <sup>1</sup>Sandia National Laboratories*

**Growth Optimization of Single Crystal Fibers from Polycrystalline Source Rods Using Laser Heated Pedestal Methods:** *Dolendra Karki<sup>1</sup>; Edward Clover Hoffman<sup>1</sup>; Paul R. Ohodnicki<sup>1</sup>; <sup>1</sup>University of Pittsburgh*

**Novel Oxide Glasses Via Non-traditional Processing:** *Adam Floyd<sup>1</sup>; Vinh Nguyen<sup>2</sup>; Daniel Rhonehouse<sup>2</sup>; Robel Bekele<sup>3</sup>; Jason Myers<sup>2</sup>; Daniel Gibson<sup>2</sup>; Shyam Bayya<sup>2</sup>; Rick Kim<sup>2</sup>; Jesse Frantz<sup>2</sup>; Jasbinder Sanghera<sup>2</sup>; <sup>1</sup>Jacobs Technology, Inc; <sup>2</sup>U.S. Naval Research Laboratory; <sup>3</sup>University Research Foundation*



# Technical Program

**Comparison of Spinel Produced by SPS and Traditional Pressing Techniques:** *Adam Floyd*<sup>1</sup>; Noor Qadri<sup>2</sup>; Bryan Sadowski<sup>1</sup>; Guillermo Villalobos<sup>2</sup>; Shyam Bayya<sup>2</sup>; Rick Kim<sup>2</sup>; Syed Qadri<sup>2</sup>; Jasbinder Sanghera<sup>2</sup>; <sup>1</sup>Jacobs Technology Inc.; <sup>2</sup>U.S. Naval Research Laboratory

**Glasses for Multiband Optics:** *Daniel Gibson*<sup>1</sup>; Vinh Nguyen<sup>2</sup>; Daniel Rhonehouse<sup>2</sup>; Adam Floyd<sup>2</sup>; Shyam Bayya<sup>2</sup>; Jasbinder Sanghera<sup>2</sup>; <sup>1</sup>563882; <sup>2</sup>U.S. Naval Research Laboratory

**Study of Silica Glass Structural Properties under Compression Shockwave Using Reactive Force Field:** *Ashish Yadav*<sup>1</sup>; Vaibhav Bihani<sup>1</sup>; N.M. Anoop Krishnan<sup>1</sup>; <sup>1</sup>Indian Institute of Technology (IIT), Delhi

**Chalcogenides and Chalcopyrites; Growth of Multinary Cystals and Glasses for Lasers and Hyperspectral Imagers:** *Narsingh Singh*; Ian Emge<sup>1</sup>; Pooja Gautam<sup>2</sup>; Krishna Machuga<sup>1</sup>; Fow-Sen Choa<sup>1</sup>; Bradley Arnold<sup>1</sup>; Lisa Kelly<sup>1</sup>; Brian Cullum<sup>1</sup>; Raghav Rai<sup>3</sup>; <sup>1</sup>University of Maryland Baltimore County; <sup>2</sup>Indian Institute of Technology, BHU; <sup>3</sup>Applied Novel Devices Inc

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## FUNDAMENTALS AND CHARACTERIZATION

### Grain Boundaries, Interfaces, and Surfaces in Ceramics: Fundamental Structure—Property—Performance Relationships — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division

**Program Organizers:** Rheinheimer Wolfgang, Forschungszentrum Jülich; Catherine Bishop, University of Canterbury; Shen Dillon, University of California, Irvine; Ming Tang, Rice University; John Blendell, Purdue University; Wayne Kaplan, Technion - Israel Institute of Technology; Melissa Santala, Oregon State University

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On-Demand Room 7 | MS&T On Demand

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#### Invited

**Interface Migration: From Grain Boundary Structure to Microstructure Evolution:** *David Srolovitz*<sup>1</sup>; Jian Han<sup>1</sup>; Marco Salvalaglio<sup>2</sup>; <sup>1</sup>City University of Hong Kong; <sup>2</sup>TU Dresden

#### Invited

**Triggering the Catalytic Activity of SrTiO<sub>3</sub>-based Ceramics by Electric-field-assisted Treatments:** *Simone Mascotto*<sup>1</sup>; <sup>1</sup>University of Hamburg

#### Invited

**Abnormal Grain Growth in Nanocrystalline PdAu: The Case of the Fractal Fingerprint:** Raphael Zeller<sup>1</sup>; Markus Fischer<sup>1</sup>; Christian Braun<sup>2</sup>; Mingyan Wang<sup>1</sup>; Rainer Birringer<sup>2</sup>; *Carl Krill III*<sup>1</sup>; <sup>1</sup>Ulm University; <sup>2</sup>Saarland University

#### Invited

**Fast Grain-boundary Diffusion in Oxides:** *Roger De Souza*<sup>1</sup>; <sup>1</sup>RWTH Aachen University

#### Invited

**Influence of Li on Planar Defects on the Electrochemical Cycling and Diffusion of Li in Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub>:** Torben Erichsen<sup>1</sup>; Cynthia Volkert<sup>1</sup>; <sup>1</sup>University of Goettingen

**On the Role of Plasticity in High Heating Rate Sintering: Does Flash Sintering Involve Plastic Flow?:** *Rheinheimer Wolfgang*<sup>1</sup>; Xin Phuah<sup>2</sup>; Lukas Porz<sup>3</sup>; Michael Scherer<sup>3</sup>; Jaehun Cho<sup>2</sup>; Haiyan Wang<sup>2</sup>; <sup>1</sup>Forschungszentrum Jülich; <sup>2</sup>Purdue University; <sup>3</sup>TU Darmstadt

**3-D Quantification of Grain Boundary Defect Chemistry Using TEM + APT:** *Brian Gorman*<sup>1</sup>; <sup>1</sup>Colorado School of Mines

**Geometrical Asymmetry Enabled Low Field Nucleation and Manipulation of Skyrmion at Magnetic Domain Boundaries in a Centro-symmetric Magnet:** *Binbin Wang*<sup>1</sup>; Po-kuan Wu<sup>1</sup>; Nuria Bagues<sup>1</sup>; Qiang Zheng<sup>2</sup>; Jiaqiang Yan<sup>2</sup>; Mohit Randeria<sup>1</sup>; David McComb<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Oak Ridge National Laboratory

**Dislocation and Grain Boundary Interaction in Oxides: Slip Transmission or Cracking?:** *Kuan Ding*<sup>1</sup>; Wolfgang Rheinheimer<sup>2</sup>; Wenzhen Xia<sup>3</sup>; Christian Dietz<sup>1</sup>; Enrico Bruder<sup>1</sup>; Karsten Durst<sup>1</sup>; Atsutomo Nakamura<sup>4</sup>; Xufei Fang<sup>1</sup>; <sup>1</sup>TU Darmstadt; <sup>2</sup>Forschungszentrum Jülich; <sup>3</sup>Max-Planck-Institut für Eisenforschung; <sup>4</sup>Nagoya University

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## FUNDAMENTALS AND CHARACTERIZATION

### High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II — On-Demand Oral Presentations

**Sponsored by:** TMS Alloy Phases Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Michael Gao, National Energy Technology Laboratory; Xingbo Liu, West Virginia University; Peter Liaw, University of Tennessee; Jian Luo, University of California, San Diego; Yiquan Wu, Alfred University; Yu Zhong, Worcester Polytechnic Institute; Mitra Taheri, Johns Hopkins University; Amy Clarke, Colorado School of Mines

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On-Demand Room 7 | MS&T On Demand

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#### Keynote

**Recreate New Life of the Periodic Table: High-entropy Alloys:** *Jien-Wei Yeh*<sup>1</sup>; <sup>1</sup>National Tsing Hua University

#### Invited

**Oxidation Behavior of Concentrated Refractory Alloys:** *Todd Butler*<sup>1</sup>; Tinuade Daboiku<sup>1</sup>; Oleg Senkov<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory

#### Invited

**The Role of Composition and Static Displacements on Phase Stability of BCC High Entropy Alloys:** German Samolyuk<sup>1</sup>; Yuri Osetsky<sup>1</sup>; Malcolm Stocks<sup>1</sup>; *James Morris*<sup>2</sup>; <sup>1</sup>Oak Ridge National Lab; <sup>2</sup>Ames Laboratory

#### Invited

**Designing High-entropy Intermetallics: Machine Learning Models and Validation:** *Joseph Poon*<sup>1</sup>; Jie Qi<sup>1</sup>; <sup>1</sup>University of Virginia

#### Invited

**Enhanced Oxidation Resistance of (Mo95W5)85Ta10(TiZr)5 Refractory Metal Multi-principal Element Alloy Up to 1300°C:** *Ranran Su*<sup>1</sup>; Hongliang Zhang<sup>2</sup>; Gaoyuan Ouyang<sup>3</sup>; Longfei Liu<sup>2</sup>; Jun Cui<sup>3</sup>; Duane Johnson<sup>3</sup>; John Perepezko<sup>2</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>Department of Materials Science and Engineering, University of Wisconsin-Madison; <sup>3</sup>Ames Laboratory, U.S. Department of Energy at Iowa State University

**Invited**

**Ultrahigh-strength and Ductile High-entropy Alloys with Coherent Nano-lamellar Architectures:** *Zengbao Jiao*<sup>1</sup>; <sup>1</sup>The Hong Kong Polytechnic University

**Invited**

**Exploring the Chemical and Structural Phase Space of High Entropy Alloys with Ab Initio Calculations and Machine Learning Potentials:** *Fritz Koermann*<sup>1</sup>; <sup>1</sup>Tu Delft

**Invited**

**Local Ordering and Defect Evolution in Body-centered Cubic (BCC) Multi-principal Element Alloys:** *Shijun Zhao*<sup>1</sup>; <sup>1</sup>City University of Hong Kong

**Invited**

**FeNiMnAl(Cr) Multi-principal Component Alloys:** *Ian Baker*<sup>1</sup>; <sup>1</sup>Dartmouth College

**Invited**

**Creep Performance of Various Single Phase FCC CoCrFeNi Family of High Entropy Alloys:** *Kyle Rozman*<sup>1</sup>; *Martin Detrois*<sup>1</sup>; *Paul Jablonski*<sup>1</sup>; *Michael Gao*<sup>1</sup>; *Jeffery Hawk*<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

**Invited**

**Microstructure and Mechanical Properties of Hf-27Ta and Hf-21Ta-21X (X is Nb, Mo or W) Alloys:** *Oleg Senkov*<sup>1</sup>; *Tinuade Daboiku*<sup>1</sup>; *Todd Butler*<sup>2</sup>; *Michael Titus*<sup>2</sup>; *Noah Philips*<sup>3</sup>; *Eric Payton*<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>Purdue University; <sup>3</sup>ATI Specialty Alloys and Components

**Invited**

**Tuning Mechanical Metastability in FeMnCo Medium Entropy Alloys:** *S.L. Wei*<sup>1</sup>; *M. Xu*<sup>1</sup>; *James LeBeau*<sup>1</sup>; *C. Tasan*<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**Invited**

**Ab Initio Modeling on the Elastic Properties of Al-Co-Cr-Fe-Ni High Entropy Alloys: A Case Study with FCC Phase:** *Songge Yang*<sup>1</sup>; *Yu Zhong*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**Invited**

**Theories for Predicting Simple Solid Solution High-entropy Alloys: Classification, Accuracy, and Important Factors Impacting Accuracy:** *Jian-Hong Li*<sup>1</sup>; *Ming-Hung Tsa*<sup>2</sup>; *An-Chen Fan*<sup>1</sup>; <sup>1</sup>National Chung Hsing University

**Thermal Conductivity Reduction in (Zr<sub>0.25</sub>Ta<sub>0.25</sub>Nb<sub>0.25</sub>Ti<sub>0.25</sub>)C High Entropy Carbide from Extrinsic Lattice Defects:** *Cody Dennett*<sup>1</sup>; *Fei Wang*<sup>2</sup>; *Bai Cui*<sup>2</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>University of Nebraska-Lincoln

**Interstitial Induced Transformations in Nb-Ti Alloys:** *Ravit Silverstein*<sup>1</sup>; *Anirudh Natarajan*<sup>1</sup>; *Raphaële Clément*<sup>1</sup>; *Anton Van der Ven*<sup>1</sup>; *Carlos Levi*<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

**A Novel Soft-magnetic Single-phase B2-ordered Multi-principal Element Alloy:** *Youxiong Ye*<sup>1</sup>; *Scott Lish*<sup>1</sup>; *Liubin Xu*<sup>2</sup>; *Markus Wittmann*<sup>2</sup>; *Haixuan Xu*<sup>2</sup>; *Ian Baker*<sup>1</sup>; <sup>1</sup>Dartmouth College; <sup>2</sup>Department of Materials Science and Engineering

**Deformation of Refractory Multi-principal Element Alloy Nanowires:** *Shuozhi Xu*<sup>1</sup>; *Yanqing Su*<sup>2</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>Utah State University

**Understanding the Nature of Passivation Film of a TRIP Fe<sub>39</sub>Mn<sub>20</sub>Co<sub>20</sub>Cr<sub>15</sub>Si<sub>5</sub>Al<sub>1</sub> (at.%) High Entropy Alloy in 3.5 wt.% NaCl Solution:** *Pranshul Varshney*<sup>1</sup>; *Nilesh Kumar*<sup>1</sup>; <sup>1</sup>University of Alabama-Tusaloosa

**ENERGY**

**Hybrid Organic—Inorganic Materials for Alternative Energy — On-Demand Hybrid Organic—Inorganic Materials for Alternative Energy**

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Andrei Jitianu, Lehman College, City University of New York; Lisa Klein, Rutgers University; Lia Stanciu, Purdue University; Mihaela Jitianu, William Paterson University

**Friday AM | October 22, 2021**

**On-Demand Room 6 | MS&T On Demand**

**Invited**

**Challenges and Opportunities of Polymer Nanodielectrics for Electric Energy Storage:** *Lei Zhu*<sup>1</sup>; <sup>1</sup>Case Western Reserve University

**Invited**

**Proton-conducting Oxides for Energy Conversion:** *Chuancheng Duan*<sup>1</sup>; <sup>1</sup>Kansas State University

**Application of Hybrid Photoanode Structures in Dye Sensitized Solar Cells (DSSCs):** *Pawel Jarka*<sup>1</sup>; *Tomasz Tanski*<sup>1</sup>; *Wiktor Matysiak*<sup>1</sup>; *Aleksandra Drygala*<sup>1</sup>; <sup>1</sup>Silesian University of Technology

**Invited**

**Grain Boundary Passivation for Enhancing Stability of Hybrid Perovskite Solar Cells:** *Chang-Yong Nam*<sup>1</sup>; <sup>1</sup>Brookhaven National Laboratory

**Invited**

**Oxide Nanosheets in Hybrid Structures:** *Alp Sehirliglu*<sup>1</sup>; *Kevin Pachuta*<sup>1</sup>; *Maria Escamilla*<sup>2</sup>; *Katelynn Edgehouse*<sup>1</sup>; *Emily Pentzer*<sup>2</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>Texas A&M

**Invited**

**Translational Research in Energy Storage: Opportunities for Flow Battery Science:** *James McKone*<sup>1</sup>; *Tejal Sawant*<sup>1</sup>; *Becca Segel*<sup>1</sup>; *Zachary Parr*<sup>1</sup>; *Carissa Yim*<sup>1</sup>; *Thomas Henry*<sup>1</sup>; <sup>1</sup>University of Pittsburgh

**Enhancement of Viscoelastic Properties of MR-elastomer by Iron Particle Chain Structures for Adaptive Vibration Control:** *Narongdet Sulatchaneenopdon*<sup>1</sup>; *Hyoung-Won Son*<sup>1</sup>; *Anak Khantachawana*<sup>2</sup>; *Jon Garcia-Barrueta*<sup>3</sup>; *Maria Jesús Elejabarrieta*<sup>3</sup>; *Tsutomu Takahashi*<sup>1</sup>; *Hisayuki Suematsu*<sup>1</sup>; *Koichi Niihara*<sup>1</sup>; *Tadachika Nakayama*<sup>1</sup>; <sup>1</sup>Nagaoka University of Technology; <sup>2</sup>King Mongkut's University of Technology; <sup>3</sup>University of Deusto

# Technical Program

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## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III — On-Demand Oral Session I

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 7 | MS&T On Demand**

**Session Chairs:** Jon Molina-Aldareguia, Imdea Materials Institute; M Arul Kumar, Los Alamos National Laboratory

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#### Invited

**Yield Point Phenomena in Single Crystal BCC and FCC Metals:** *David Fullwood<sup>1</sup>; Josh Tsai<sup>1</sup>; Tristan Russell<sup>1</sup>; Guowei Zhou<sup>2</sup>; Robert Wagoner<sup>3</sup>; Eric Homer<sup>1</sup>; <sup>1</sup>Brigham Young University; <sup>2</sup>Shanghai Jiao Tong University; <sup>3</sup>Ohio State University*

**Two-scale Simulation of Plastic eformation in BCC Metals: Combination of Atomistic Simulation and Dislocation Dynamics:** *Sergei Starikov<sup>1</sup>; Vasily Tseplyaev<sup>2</sup>; Matous Mrovec<sup>1</sup>; <sup>1</sup>ICAMS, Ruhr University Bochum; <sup>2</sup>Grunberg Institut and Institute for Advanced Simulation*

**Transformation-induced Plasticity in Omega Titanium:** *Amir Hassan Zahiri<sup>1</sup>; Jamie Ombogo<sup>1</sup>; Tengfei Ma<sup>1</sup>; Pranay Chakraborty<sup>1</sup>; Lei Cao<sup>1</sup>; <sup>1</sup>University Of Nevada Reno*

**Combining DICTRA Simulations with In-situ TEM Experiments to Optimize Metallic Powder Heat Treatments:** *Kyle Tsaknopoulos<sup>1</sup>; Matthew Gleason<sup>1</sup>; Grace Fitzpatrick-Schmidt<sup>1</sup>; Danielle Cote<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute*

**Interactions between Dislocations and 3D Interfaces in a Cu/Nb System:** *Shuozhi Xu<sup>1</sup>; Justin Cheng<sup>2</sup>; Zezhou Li<sup>2</sup>; Nathan Mara<sup>2</sup>; Irene Beyerlein<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara; <sup>2</sup>University of Minnesota, Twin Cities*

**Automated Laue Pattern Analysis for Bragg Coherent Diffraction Imaging:** *Yueheng Zhang<sup>1</sup>; Anthony Rollett<sup>1</sup>; Robert Suter<sup>1</sup>; <sup>1</sup>Carnegie Mellon University*

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## FUNDAMENTALS AND CHARACTERIZATION

### Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales III — On-Demand Oral Session II

**Program Organizers:** Mariyappan Arul Kumar, Los Alamos National Laboratory; Irene Beyerlein, University of California, Santa Barbara; Levente Balogh, Queen's University; Caizhi Zhou, University of South Carolina; Lei Cao, University of Nevada; Josh Kacher, Georgia Institute of Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 7 | MS&T On Demand**

**Session Chairs:** Deep Choudhuri, New Mexico Institute of Mining and Technology; D Biswas, IIT Kharagpur

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#### Invited

**Extension Twin Induced Strain Hardening and Texture Evolution in AM30 Alloy: Experiments and Crystal Plasticity Modelling:** *Somjeet Biswas<sup>1</sup>; <sup>1</sup>India Institute of Technology Kharagpur*

#### Invited

**An Integrated Numerical Approach to Investigate the Effect of Grain-scale Heterogeneities on the Anisotropy of Polycrystalline Metals:** *Kyung Mun Min<sup>1</sup>; Hyukjae Lee<sup>1</sup>; Heung Nam Han<sup>1</sup>; Myoung-Gyu Lee<sup>1</sup>; <sup>1</sup>Seoul National University*

#### Invited

**Deformation of Lamellar FCC-B2 Nanostructures Containing Kurdjumov-Sachs Interfaces: Relation between Interfacial Structure and Plasticity:** *Deep Choudhuri<sup>1</sup>; Srivilliputhur Srinivasan<sup>2</sup>; Rajiv Mishra<sup>2</sup>; <sup>1</sup>New Mexico Institute of Mining and Technology; <sup>2</sup>University of North Texas*

**Formation of {112  $\bar{2}$ } Contraction Twins in Titanium through Reversible Martensitic Phase Transformation:** *Amir Hassan Zahiri<sup>1</sup>; Jamie Ombogo<sup>1</sup>; Lei Cao<sup>1</sup>; <sup>1</sup>University of Nevada Reno*

**Modeling the Composition of Primary Carbides in the System Ni-11.5Cr-5Co-3.6Al-4.5Ti-7W-0.8Mo-0.06C:** *Alexander Glotka<sup>1</sup>; <sup>1</sup>Zaporizhzhia Polytechnic National University*

**A Microstructural Model for Creep-fatigue Damage in Grade 91 Steel:** *Ajey Venkataraman<sup>1</sup>; Andrea Rovinelli<sup>1</sup>; Mark Messner<sup>1</sup>; <sup>1</sup>Argonne National Laboratory*

**Design of an Austenitic Steel Weldment System Using ICME:** *Daniel Bechetti<sup>1</sup>; Paul Lambert<sup>1</sup>; Matthew Sinfield<sup>1</sup>; Charles Fisher<sup>1</sup>; <sup>1</sup>Naval Surface Warfare Center, Carderock Division*

**Phase-field Simulations of Translation of Grains in Strain-energy-driven Grain Growth:** *Guanglong Huang<sup>1</sup>; David Montiel<sup>1</sup>; Matthew Higgins<sup>1</sup>; Jiwoong Kang<sup>1</sup>; Ning Lu<sup>1</sup>; Ashwin Shahani<sup>1</sup>; Katsuyo Thornton<sup>1</sup>; <sup>1</sup>University of Michigan*

## SPECIAL TOPICS

### Late News Poster Session — On-Demand Additive Manufacturing Poster Session

Friday AM | October 22, 2021  
 On-Demand Poster Hall | MS&T On Demand

**Fabrication of Doped  $\beta$ -tricalcium Phosphate Bioceramics by Robocasting for Bone Repair Applications:** *Nicolas Somers*<sup>1</sup>; Florian Jean<sup>1</sup>; Marie Lasgorceix<sup>1</sup>; Anthony Thuault<sup>1</sup>; Fabrice Petit<sup>2</sup>; Sandra Balvay<sup>3</sup>; Christelle Der Loughian<sup>3</sup>; Claire Gaillard<sup>3</sup>; Laurent Gremillard<sup>3</sup>; Anne Leriche<sup>1</sup>; <sup>1</sup>LMCPA/UPHF; <sup>2</sup>Belgian Ceramic Research Center; <sup>3</sup>I2B/Mateis-INSa Lyon

**Hybrid Additive/Subtractive System of Ceramic Materials: Investigation of Powder, Process and Innovative Post-treatments:** *Qirong Chen*<sup>1</sup>; Enrique Juste<sup>1</sup>; Marie Lasgorceix<sup>2</sup>; Fabrice Petit<sup>1</sup>; Anne Leriche<sup>2</sup>; <sup>1</sup>Belgium Ceramic Research Centre; <sup>2</sup>Laboratoire des Matériaux Céramiques et Procédés Associés

**Scanning Strategies Investigation for Powder Bed Selective Laser Processing of Alumina:** *Mohamed Abdelmoula*<sup>1</sup>; Giovanni Urruth<sup>2</sup>; Gökhan Küçüktürk<sup>1</sup>; Enrique Juste<sup>3</sup>; Fabrice Petit<sup>3</sup>; <sup>1</sup>Gazi University; <sup>2</sup>Marion Technologies; <sup>3</sup>Belgium Ceramic Research Center

**Texture Evolution during the High Temperature Heat Treatment of Additively Manufactured IN718:** *Selda Nayir*<sup>1</sup>; Bertrand Max<sup>2</sup>; Simon Perusin<sup>2</sup>; Todd Palmer<sup>1</sup>; <sup>1</sup>Pennsylvania State University; <sup>2</sup>IRT Saint Exupéry, Institut de Recherche Technologique

## SPECIAL TOPICS

### Late News Poster Session — On-Demand Artificial Intelligence Poster Session

Friday AM | October 22, 2021  
 On-Demand Poster Hall | MS&T On Demand

**LSTM Model to Predict Low-cycle Fatigue in IN718:** *Jacob Keesler-Evans*<sup>1</sup>; Ansan Pokharel<sup>1</sup>; Terence Musho<sup>1</sup>; <sup>1</sup>West Virginia University

## SPECIAL TOPICS

### Late News Poster Session — On-Demand Fundamentals and Characterization Poster Session

Friday AM | October 22, 2021  
 On-Demand Poster Hall | MS&T On Demand

**Extrinsic Size Effects on Fracture Behaviour of Copper:** *Hrushikesh Sahasrabudhe*<sup>1</sup>; Anirban Patra<sup>1</sup>; Nagamani Jaya Balila<sup>1</sup>; <sup>1</sup>India Institute of Technology Bombay

**Microstructural Conditioning to Reveal Prior Austenitic Grain Using the Oxidation Method:** David Fernandez-Sanchez<sup>1</sup>; Alexis Gallegos-Perez<sup>1</sup>; Octavio Vázquez-Gómez<sup>1</sup>; Pedro Garnica-Gonzalez<sup>1</sup>; Hector Vergara-Hernandez<sup>1</sup>; *Antonio Oliver-Reynoso*<sup>2</sup>; <sup>1</sup>Tecnológico Nacional de México / I.T. Morelia; <sup>2</sup>Tecnológico Nacional de México / I.T. Morelia

**Nanoindentation studies on Friction Stir Processed Dual Phase High Entropy Alloy:** *Neelam Meena*<sup>1</sup>; Gourav Rao<sup>2</sup>; Nithyanand Prabhu<sup>1</sup>; <sup>1</sup>IIT BOMBAY; <sup>2</sup>Naval Materials Research Laboratory

## PROCESSING AND MANUFACTURING

### Light Metal Technology — On-Demand Oral Presentations

*Sponsored by:* TMS Titanium Committee

**Program Organizers:** Xiaoming Wang, Purdue University; Yufeng Zheng, University of Nevada-Reno

Friday AM | October 22, 2021  
 On-Demand Room 12 | MS&T On Demand

**Surface Modification of Steel Shells to Reduce the Use of Release Agents in Twin Roll Casting of Aluminum Alloys:** *Martin Lauth*<sup>1</sup>; Alexander Nienhaus<sup>2</sup>; Hanno Paschke<sup>3</sup>; Mirko Schaper<sup>1</sup>; Olexandr Grydin<sup>1</sup>; <sup>1</sup>University of Paderborn; <sup>2</sup>TU Braunschweig; <sup>3</sup>Fraunhofer Institute

**EPSC Model with Back Stress Development to Capture Multi-strain-path Behavior of AA6016-T4:** *Rishabh Sharma*<sup>1</sup>; Dane Sargeant<sup>1</sup>; Sowmya Daroju<sup>2</sup>; Marko Kenezevic<sup>2</sup>; Michael Miles<sup>1</sup>; David Fullwood<sup>1</sup>; <sup>1</sup>Brigham Young University; <sup>2</sup>University of New Hampshire

**In-situ Observation the Growth of Fe-rich Phases during Al Alloys Solidification:** *Yuliang Zhao*<sup>1</sup>; <sup>1</sup>Dongguan University of Technology

## CERAMIC AND GLASS MATERIALS

### Manufacturing and Processing of Advanced Ceramic Materials — On-Demand Advanced Manufacturing Process of Ceramics

*Sponsored by:* ACeRS Manufacturing Division

**Program Organizers:** Bai Cui, University of Nebraska-Lincoln; James Hemrick, Oak Ridge National Laboratory; Mike Alexander, Allied Mineral Products; Eric Faierson, Quad City Manufacturing Laboratory / Western Illinois University; Keith DeCarlo, Blasch Precision Ceramics

Friday AM | October 22, 2021  
 On-Demand Room 4 | MS&T On Demand

**Session Chairs:** Tatsuki Ohji, National Institute of Advanced Industrial Science and Technology; Bai Cui, University of Nebraska-Lincoln

## Invited

**The Future of Manufacturing in Energy-intensive Industries:** *William Lee*<sup>1</sup>; Michael Rushton<sup>1</sup>; Simon Middleburgh<sup>1</sup>; Phylis Makurunjé<sup>1</sup>; <sup>1</sup>Bangor University



# Technical Program

## Invited

**Making Pre-stressed Ceramics with High Strength and High Damage Tolerance:** Yiwang Bao<sup>1</sup>; Fenghua Kuang<sup>1</sup>; Yi Sun<sup>2</sup>; Yueming Li<sup>2</sup>; Detian Wan<sup>1</sup>; Zongyang Shen<sup>2</sup>; Delong Ma<sup>1</sup>; *Lingfeng He*<sup>3</sup>; <sup>1</sup>China Building Materials Academy; <sup>2</sup>Jingdezhen Ceramic Institute; <sup>3</sup>Idaho National Laboratory

## Invited

**Progress of Silicon Nitride: Processing, Structure and Property:** *Tatsuki Ohji*<sup>1</sup>; You Zhou<sup>1</sup>; Hiroyuki Miyazaki<sup>1</sup>; Hideki Hyuga<sup>1</sup>; Kiyoshi Hirao<sup>1</sup>; <sup>1</sup>National Institute of Advanced Industrial Science and Technology

## Invited

**Issues Related to the Manufacturing and Processing of Refractory Ceramic Materials:** *James Hemrick*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**Comparison of Microstructural Evolution of Hydroxyapatite Powder Sintered by Microwave, SPS and Conventional Sintering:** *Anne Leriche*<sup>1</sup>; Pierre Lefevre<sup>1</sup>; Védi Dupont<sup>2</sup>; Diana Vitiello<sup>3</sup>; Hamza Karouti<sup>3</sup>; Anthony Thuault<sup>1</sup>; David Smith<sup>3</sup>; Stéphane Hocquet<sup>2</sup>; <sup>1</sup>UPHF - LMCPA; <sup>2</sup>BCRC; <sup>3</sup>IRCIER Limoges

**Luminescence Thermometry - Striving a Breakthrough:** *Eugeniusz Zych*<sup>1</sup>; Paulina Bolek<sup>1</sup>; Malgorzata Sójka<sup>1</sup>; Dagmara Kulesza<sup>1</sup>; Joanna Trojan-Piegha<sup>1</sup>; <sup>1</sup>University of Wrocław

**Leveraging Computational Thermodynamics for Guiding SiC-ZrC Chemical Vapor Deposition Process Development:** *Benjamin Lamm*<sup>1</sup>; Jian Peng<sup>2</sup>; Jake McMurray<sup>2</sup>; Dongwon Shin<sup>2</sup>; David Mitchell<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Materials Science and Technology Division, Oak Ridge National Laboratory

**Selective Laser Sintering of Hexagonal Barium Titanate Ceramics:** Xiang Zhang<sup>1</sup>; Fei Wang<sup>1</sup>; Zhipeng Wu<sup>1</sup>; Yongfeng Lu<sup>1</sup>; Yan Chen<sup>2</sup>; Michael Nastasi<sup>3</sup>; *Bai Cu*<sup>1</sup>; <sup>1</sup>University of Nebraska-Lincoln; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>Texas A&M University

**Chemical Vapor Deposition of Zirconium-silicon-carbon Compositions:** *David Mitchell*<sup>1</sup>; Benjamin Lamm<sup>1</sup>; Michael Lance<sup>1</sup>; Kevin Cooley<sup>1</sup>; Ercan Cakmak<sup>1</sup>; Todd Groff<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**A Novel Room-temperature Synthesis Technique for Producing High-density Electroceramic Composites:** *Evan Smith*<sup>1</sup>; Rick Ubic<sup>1</sup>; <sup>1</sup>Boise State University

**Aqueous Colloidal Processing of WC Based Materials with Alternative Metals as Sintering Aids or Binder:** *Antonio Javier Sanchez-Herencia*<sup>1</sup>; Macarena Garcia-Ayala<sup>1</sup>; Begoña Ferrari<sup>1</sup>; Jose Ygnacio Pastor<sup>2</sup>; <sup>1</sup>Institute for Ceramic and Glass; <sup>2</sup>ETSI Caminos-UPM

**Spark Plasma Joining of HfB<sub>2</sub>-ZrB<sub>2</sub>-SiC Composites Using Ni as a Filler:** *Shipra Bajpai*<sup>1</sup>; Alok Bhaduria<sup>1</sup>; T. Venkateswaran<sup>2</sup>; Sudhanshu Singh<sup>1</sup>; Kantesh Balani<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Kanpur; <sup>2</sup>Vikram Sarabhai Space Centre/ISRO

**Pressureless Sintered SiC Formed via Thermoplastic Fugitive Binders for High-temperature Applications:** *Rodrigo Orta Guerra*<sup>1</sup>; Olivia Brandt<sup>1</sup>; Rodney Trice<sup>1</sup>; Jeffrey Youngblood<sup>1</sup>; <sup>1</sup>Purdue University

**Development Calcium Doped La(Cr<sub>0.2</sub>Co<sub>0.2</sub>Fe<sub>0.2</sub>Mn<sub>0.2</sub>Ni<sub>0.2</sub>)O<sub>3</sub> High Entropy Perovskite Oxides:** *Sai Ram Gajjala*<sup>1</sup>; Rasit Koc<sup>1</sup>; <sup>1</sup>Southern Illinois University

**Mechanical Properties of La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>/ZrO<sub>2</sub> Composites Prepared by Coating of ZrO<sub>2</sub> Sol:** *Bong-Gu Kim*<sup>1</sup>; Hyun-Hee Choi<sup>2</sup>; GuanLin Lyu<sup>2</sup>; JangHyeok Pyeon<sup>1</sup>; Jung-Hun Son<sup>2</sup>; SeungCheol Yang<sup>1</sup>; Yeon-Gill Jung<sup>1</sup>; <sup>1</sup>Department of Materials Convergence and System Engineering of Changwon National University; <sup>2</sup>Changwon national university

**Dispersion Studies of Alumina Toughened Zirconia Powders for Direct Ink Writing Applications:** *Berfu Goeksel*<sup>1</sup>; Erin Koos<sup>1</sup>; Bart Van Meerbeek<sup>1</sup>; Jozef Vleugels<sup>1</sup>; Annabel Braem<sup>1</sup>; <sup>1</sup>KU Leuven

**Analysis of Crystal Structure in Calcium and Strontium Hexaborides with Lithium Popancies:** *Alan Hirales*<sup>1</sup>; Olivia Graeve<sup>1</sup>; <sup>1</sup>University of California San Diego

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## ARTIFICIAL INTELLIGENCE

### Materials Informatics for Images and Multi-dimensional Datasets — On-Demand Oral Presentations

**Sponsored by:** ACeRS Basic Science Division, ACeRS Electronics Division

**Program Organizers:** Amanda Krause, University of Florida; Alp Sehirlioglu, Case Western Reserve University; Daniel Ruscitto, General Electric

**Friday AM | October 22, 2021**  
**On-Demand Room 2 | MS&T On Demand**

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## Invited

**Training Deep-learning Models with 3D Microstructure Images to Predict Location-dependent Mechanical Properties in Additive Manufacturing:** *Ashley Spear*<sup>1</sup>; Carl Herriott<sup>1</sup>; <sup>1</sup>University of Utah

## Invited

**Understanding Degradation and Failure Mechanisms by Multiscale and Multiresolution Electron Microscopy:** *Josh Kacher*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

## Invited

**Graph Neural Networks for an Accurate and Interpretable Prediction of the Properties of Polycrystalline Materials:** Minyi Dai<sup>1</sup>; Mehmet Demirel<sup>1</sup>; Yingyu Liang<sup>1</sup>; *Jiamian Hu*<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

## Invited

**Open-source Hyper-dimensional Materials Analytics Using Hyperspy:** *Joshua Taillon*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

## Invited

**Machine Learning Ferroelectrics: Bayesianity, Parsimony, and Causality:** *Sergei Kalinin*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**Multivariate Statistical Analysis (MVSA) for Hyperspectral Images:** *Chuong Nguyen*<sup>1</sup>; Alp Manavbasi<sup>1</sup>; <sup>1</sup>Novelis

## FUNDAMENTALS AND CHARACTERIZATION

### Materials vs Minerals: Bridging the Gap between Materials Science and Earth and Planetary Science — On-Demand Oral Presentations

**Sponsored by:** ACerS

**Program Organizers:** Jessica Rimsza, Sandia National Laboratories; Krishna Muralidharan, The University of Arizona; Thomas, The University of Arizona

**Friday AM | October 22, 2021**  
**On-Demand Room 7 | MS&T On Demand**

**Coupling Aberration Corrected STEM and DFT to Determine the Crystal Chemistry of Hibonite for Application to Early Solar System Thermodynamics:** *Pierre-marie Zanetta*<sup>1</sup>; Venkat Manga<sup>2</sup>; Yao-Jen Chang<sup>2</sup>; Tarunika Ramprasad<sup>3</sup>; Thomas Zega<sup>2</sup>; <sup>1</sup>University of Arizona; <sup>2</sup>Lunar and Planetary Laboratory, The University of Arizona; <sup>3</sup>The University of Arizona

**Investigation of Variable Manganese and Nickel Content on Ductile Iron Castings Utilizing Ionic Liquids Isolated Iron and Bosch Carbon:** *Blake Stewart*<sup>1</sup>; Haley Doude<sup>1</sup>; Jennifer Edmunson<sup>2</sup>; Eric Fox<sup>2</sup>; Morgan Abney<sup>3</sup>; Paul Hintze<sup>2</sup>; Jeffrey Mehan<sup>2</sup>; Hongjoo Rhee<sup>1</sup>; <sup>1</sup>Mississippi State University; <sup>2</sup>Marshall Space Flight Center; <sup>3</sup>Langley Research Center

**Modeling Thermodynamics of Condensation of Fe-Ti-bearing Byroxenes Relevant to the Early Solar System:** *Venkateswara Manga*<sup>1</sup>; Thomas Zega<sup>1</sup>; <sup>1</sup>Lunar and Planetary Laboratory/University of Arizona

**Chemical Pathways for Formation of Carbon Nanostructures from Graphite: Implications for Circumstellar and Solar-system Carbon:** *Abhishek Thakur*<sup>1</sup>; Krishna Muralidharan<sup>1</sup>; Thomas Zega<sup>1</sup>; Lucy Ziurys<sup>1</sup>; <sup>1</sup>University of Arizona

## NANOMATERIALS

### Mechanistic Insights into the Synergistic Properties of Nanocomposites — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Bioceramics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Vuk Uskokovic, University of California; Dragan Uskokovic, Institute of Technical Sciences of the Serbian Academy of Sciences and Arts

**Friday AM | October 22, 2021**  
**On-Demand Room 11 | MS&T On Demand**

#### Invited

**Laser-deposited Films Containing Silver Nanoparticles for Antimicrobial Applications:** *Roger Narayan*<sup>1</sup>; <sup>1</sup>University of North Carolina

## NANOMATERIALS

### Mechanistic Insights into the Synergistic Properties of Nanocomposites — On-Demand Poster Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Bioceramics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Vuk Uskokovic, University of California; Dragan Uskokovic, Institute of Technical Sciences of the Serbian Academy of Sciences and Arts

**Friday AM | October 22, 2021**  
**On-Demand Poster Hall | MS&T On Demand**

**Synergistic Effect of SiC and Carbon-based Flame Retardant Additives on Mechanical and Thermal Stability of Polypropylene Based Nanocomposites:** *Shruti Dubey*<sup>1</sup>; Kantesh Balani<sup>1</sup>; J. Ramkumar<sup>1</sup>; Surya Singh<sup>1</sup>; <sup>1</sup>Indian Institute of Technology

## MODELING

### Multi Scale Modeling of Microstructure Deformation in Material Processing — On-Demand Oral: Multi Scale Modeling of Microstructure Deformation in Material Processing

**Sponsored by:** AIST Metallurgy—Processing, Products and Applications Technology Committee

**Program Organizers:** Lukasz Madej, AGH University of Science and Technology; Jaimie Tiley, Oak Ridge National Laboratory; Muszka Krzysztof, AGH University of Science and Technology; Danuta Szeliga, AGH University of Science and Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 10 | MS&T On Demand**

**Session Chair:** Krzysztof Muszka, AGH University

**Hot Deformation Microstructure and Processing Map of Cast Ni-based Superalloy IN-100:** *Yusaku Hasebe*<sup>1</sup>; Takehito Hagisawa<sup>2</sup>; Satoru Ohsaki<sup>2</sup>; Kazuya Kubo<sup>2</sup>; Cheng Yang<sup>2</sup>; Kenta Aoyagi<sup>2</sup>; Kenta Yamanaka<sup>2</sup>; Akihiko Chiba<sup>2</sup>; <sup>1</sup>The Japan Steel Works LTD; <sup>2</sup>Japan

**Enabling Accurate Coarse-grained Atomistic Simulation of Defect Behavior in Random Alloys:** *Kevin Chu*<sup>1</sup>; Adrian Diaz<sup>2</sup>; Youping Chen<sup>3</sup>; David McDowell<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>University of Florida

**Numerical Studies of the Effect of Phase Stability on the Deformation Behavior of FeMnNiCoMo High Entropy Alloy:** *Kamil Cichocki*<sup>1</sup>; Tomasz Koziel<sup>1</sup>; Grzegorz Cios<sup>1</sup>; Lukasz Madej<sup>1</sup>; Piotr Bala<sup>1</sup>; *Krzysztof Muszka*<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology

**The Role of the Initial Digital Microstructure Generation Algorithm in the Cellular Automata Static Recrystallization Predictions:** *Mateusz Sitko*<sup>1</sup>; *Lukasz Madej*<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology

# Technical Program

**Sensitivity Analysis, Identification and Validation of the Stochastic Model Describing Evolution of Microstructural Parameters during Hot Forming of Metallic Materials:** *Danuta Szeliga*<sup>1</sup>; Natalia Czyżewska<sup>1</sup>; Konrad Klimczak<sup>1</sup>; Jan Kusiak<sup>1</sup>; Paweł Morkisz<sup>1</sup>; Piotr Oprocha<sup>1</sup>; Maciej Pietrzyk<sup>1</sup>; Paweł Przybyłowicz<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology

**Temperature and Texture Dependent Constitutive Modeling of AZ31 Sheet Magnesium:** *Daniel Kenney*<sup>1</sup>; Marcos Lugo<sup>1</sup>; Jared Darius<sup>1</sup>; <sup>1</sup>Liberty University - School of Engineering

**Using Martensite Crystallography to Determine Transformation: Induced Deformation of Ferrite In Dual-phase Steels:** *Vibhor Atreya*<sup>1</sup>; Cornelis Bos<sup>2</sup>; Maria Santofimia<sup>1</sup>; <sup>1</sup>Delft University of Technology; <sup>2</sup>Tata Steel R&D

**Multi Scale Modeling with Microstructure Characteristics of Martensitic Steel for Rolling Contact Fatigue Life Prediction:** *Jinheung Park*<sup>1</sup>; Kijung Lee<sup>1</sup>; Soonwoo Kwon<sup>2</sup>; Myoung-gyu Lee<sup>1</sup>; <sup>1</sup>Seoul National University; <sup>2</sup>Hyundai Motor Company

**Crystal Plasticity-based Forming Limit Prediction for Ultra-thin Bipolar Plate for Proton Exchange Membrane Fuel Cells:** *Minh Tien Tran*<sup>1</sup>; Dae Ho Lee<sup>1</sup>; Huai Wang<sup>2</sup>; Ho Won Lee<sup>3</sup>; Dong-Kyu Kim<sup>1</sup>; <sup>1</sup>University of Ulsan; <sup>2</sup>Chinese Academy of Sciences; <sup>3</sup>Korea Institute of Materials Science

**Crystal Plasticity Modeling of Twin Variant Selection in HCP Magnesium:** *Adwitiya Rao*<sup>1</sup>; Anirban Patra<sup>1</sup>; <sup>1</sup>IIT Bombay

**Study of Near Boundary Gradient Zones in an Aluminum Alloy Using Strain Gradient Crystal Plasticity and Experiments:** *Namit Patel*<sup>1</sup>; Indradev Samajdar<sup>1</sup>; Anirban Patra<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Bombay

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## NANOMATERIALS

**Nanotechnology for Energy, Environment, Electronics, Healthcare and Industry — On-Demand Oral Presentations**

**Sponsored by:** ACerS Electronics Division, TMS: Mechanical Behavior of Materials Committee

**Program Organizers:** Gary Pickrell, Virginia Tech; Navin Manjooran, Solve Technology and Research, Inc.

**Friday AM | October 22, 2021**  
**On-Demand Room 11 | MS&T On Demand**

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**Substituent Effects on the Solubility and Electronic Properties of the Cyanine Dye Cy5:** *Austin Biaggne*<sup>1</sup>; Jeunghoon Lee<sup>1</sup>; William Knowlton<sup>1</sup>; Bernard Yurke<sup>1</sup>; Lan Li<sup>1</sup>; <sup>1</sup>Boise State University

**Dissolution of Atherosclerosis Plaque in Human Coronary Artery Induced by Nanobubbles:** *Ao Li<sup>1</sup>; James Earthman<sup>2</sup>; <sup>1</sup>University of California Irvine; <sup>2</sup>UCIrvine*

**Skin-wearable PDMS-based Electronic Decals by Aerosol Jet 3D Printing:** *Jacob Brennenman<sup>1</sup>; Derya Tansel<sup>1</sup>; Gary Fedder<sup>1</sup>; Rahul Panat<sup>1</sup>; <sup>1</sup>Carnegie Mellon University*

**Targeted Disinfection of Pathogenic Bacteria Using a Nanostructured Electrocatalytic Device:** *Hammad Malik<sup>1</sup>; Rachel D'Agostini<sup>1</sup>; Eian Brightwell<sup>1</sup>; Dustin Williams<sup>1</sup>; Swomitra Mohanty<sup>1</sup>; Krista Carlson<sup>1</sup>; <sup>1</sup>University of Utah*

**Fabrication of Dendrite Structure Silver Nanowires / Polymer Nanocomposite for Transparent Flexible Pressure Sensor:** *Zhiming Shen<sup>1</sup>; Narongdet Sulatchaneenopdon<sup>1</sup>; Hyoung-Won Son<sup>1</sup>; Hisayuki Suematsu<sup>1</sup>; Tadachika Nakayama<sup>1</sup>; <sup>1</sup>Nagaoka University of Technology*

## IRON AND STEEL (FERROUS ALLOYS)

### New Frontiers in Physical Metallurgy of Steels — On-Demand Oral Presentations

**Sponsored by:** AIST: MPPA Committee, TMS Steels Committee

**Program Organizers:** Matthias Militzer, University of British Columbia; Pello Uranga, CEIT and TECNUN (University of Navarra); Jonah Klemm-Toole, Colorado School of Mines; Amy Clarke, Colorado School of Mines; Amit Behera, QuesTek Innovations LLC

**Friday AM | October 22, 2021**  
**On-Demand Room 8 | MS&T On Demand**

#### Invited

**New Approach to Producing High Alloy Steels:** *Hatem Zurob<sup>1</sup>; Zachary Detweiler<sup>2</sup>; Daniel Bullard<sup>2</sup>; <sup>1</sup>McMaster University; <sup>2</sup>Arcanum Alloys*

#### Invited

**Nanoscale Investigation of Austenite/ferrite Interfaces in Medium Carbon Fe-Mn-C Steels at Different Inter-critical Temperatures:** *Olha Nakonechna<sup>1</sup>; Fredric Danoix<sup>2</sup>; Helena Zapolsky<sup>2</sup>; Didier Huin<sup>3</sup>; Nicolas Charbonnier<sup>3</sup>; Lionel Germain<sup>4</sup>; Mohamed Gouné<sup>5</sup>; <sup>1</sup>University of Rouen Normandy; <sup>2</sup>CNRS/GPM; <sup>3</sup>ArcelorMittal research SA; <sup>4</sup>Université de Lorraine; <sup>5</sup>Université de Bordeaux*

**Austenite Decomposition during Hot-strip Rolling of Microalloyed Low-carbon Steel:** *Wing Shan Tam<sup>1</sup>; Matthias Militzer<sup>1</sup>; <sup>1</sup>The University of British Columbia*

**Austenite Decomposition in the Coarse Grain Heat Affected Zone of X80 Line Pipe Steel:** *Sabyasachi Roy<sup>1</sup>; Matthias Militzer<sup>1</sup>; Warren Poole<sup>1</sup>; <sup>1</sup>The University of British Columbia*

**Nano-precipitation and Resultant Surface Hardening by Nitriding of Ferrous Alloys:** *Goro Miyamoto<sup>1</sup>; Tadashi Furuhashi<sup>1</sup>; <sup>1</sup>Tohoku University*

**Microstructure and Toughness Correlation in High Strength Q&T Boron Steels Microalloyed with Nb and Mo:** *Irati Zurutuza<sup>1</sup>; Nerea Isasti<sup>1</sup>; Eric Detemple<sup>2</sup>; Volker Schwinn<sup>2</sup>; Hardy Mohrbacher<sup>3</sup>; Pello Uranga<sup>4</sup>; <sup>1</sup>CEIT and TECNUN (University of Navarra); <sup>2</sup>Dillinger Hüttenwerke; <sup>3</sup>NiobelCon bvba*

**Simulation of the Nitriding and Ferritic Nitrocarburizing (FNC) Processes:** *Mei Yang<sup>1</sup>; Haoxing You<sup>1</sup>; Richard Sisson<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute*

**Relationship between Fatigue Strength and Microstructure of Carburized Steel Tempered at Different Temperature:** *Takuya Kita<sup>1</sup>; Kazumasa Yasuda<sup>1</sup>; Junya Asaoka<sup>1</sup>; Goro Miyamoto<sup>2</sup>; Tadashi Furuhashi<sup>2</sup>; <sup>1</sup>Denso Corporation; <sup>2</sup>Tohoku University*

**Tribological Characterization of Silicon Stainless Steel Alloys:** *Prince Setia<sup>1</sup>; K Thomas Tharian<sup>2</sup>; T Venkateswaran<sup>2</sup>; Sudhanshu Shekhar Singh<sup>1</sup>; Shashank Shekhar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Kanpur; <sup>2</sup>Indian Space Research Organization*

## BIOMATERIALS

### Next Generation Biomaterials — On-Demand Oral Presentations

**Sponsored by:** ACerS Bioceramics Division, TMS Biomaterials Committee

**Program Organizers:** Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

**Friday AM | October 22, 2021**  
**On-Demand Room 3 | MS&T On Demand**

#### Invited

**Additive Manufacturing of Microstructured and Nanostructured Active Medical Devices:** *Roger Narayan<sup>1</sup>; <sup>1</sup>University of North Carolina*

#### Invited

**Hybrid Nanomanufacturing for Wearable Intelligence:** *Wenzhuo Wu<sup>1</sup>; <sup>1</sup>Purdue University*

#### Invited

**Calcium Silicate & Calcium Aluminate Bioactive Cements:** *Carolyn Primus<sup>1</sup>; <sup>1</sup>Primus Consulting*

#### Invited

**Bijels-derived Structures for Tissue Engineering Applications:** *Min Wang<sup>1</sup>; <sup>1</sup>University of Hong Kong*

#### Invited

**Novel Colloidal Based Biomaterials for Investigating Cellular Mechanotransduction Mechanisms:** *Ashley Brown<sup>1</sup>; <sup>1</sup>North Carolina State University and UNC Chapel Hill*

#### Invited

**Calcium Phosphate Nanoparticles as Intrinsic Inorganic Antimicrobials:** *Vuk Uskokovic<sup>1</sup>; <sup>1</sup>University of California*

#### Invited

**3D Binderjet Printing of Zirconia Based Ceramics, Innovative Processing Aspects and Challenges:** *Srimanta Barui<sup>1</sup>; Deepa Mishra<sup>1</sup>; Gowtham N H<sup>1</sup>; Bikramjit Basu<sup>1</sup>; <sup>1</sup>Indian Institute of Science Bangalore*

#### Invited

**Sustained Delivery of Anticancer and Antimicrobial Drugs through Hollow Silica Capsules as Transporters:** *Eva Krakor<sup>1</sup>; Isabel Gessner<sup>1</sup>; Sanjay Mathur<sup>1</sup>; <sup>1</sup>University of Cologne*

#### Invited

**Combating Plastic Waste Accumulation through Innovative Biodegradable Superabsorbent Polymers Used in Disposable Consumer Products:** *Jeffrey Bates<sup>1</sup>; <sup>1</sup>University of Utah*



# Technical Program

## Invited

**Light-based Nanomedicine: Multimodal Diagnostics Combined with Drug-free Therapeutics:** *Tanveer Tabish*<sup>1</sup>; Mohammed Sharahili<sup>2</sup>;

<sup>1</sup>Imperial College London; <sup>2</sup>University of Exeter

## Invited

**Addition of Antimicrobial Property to Hydroxyapatite/Collagen Bone-like Nanocomposite Utilizing Silver Nanoparticles:** *Masanori Kikuchi*<sup>1</sup>;

<sup>1</sup>National Institute for Materials Science

## Invited

**Stereolithographic Additive Manufacturing of Dental Crowns with Functionally Distributed Translucencies:** *Soshu Kiriha*<sup>1</sup>; <sup>1</sup>Osaka University

**Effects of Thermal Stress on Calcium Phosphate Glass-derived Cements for Vital Pulp Therapy:** *Jerry Howard*<sup>1</sup>; Jenna Young<sup>1</sup>; John Colombo<sup>2</sup>; Steven Naleway<sup>1</sup>; Krista Carlson<sup>1</sup>;

<sup>1</sup>University of Utah; <sup>2</sup>University of Nevada, Las Vegas

**Alginate Core Polyurethane Shape Memory Foam Composite with Antimicrobial Properties for Negative Pressure Wound Therapy:** *Emily Lazarus*<sup>1</sup>; Iris V. Rivero<sup>1</sup>; Robert Osgood<sup>1</sup>;

<sup>1</sup>Rochester Institute of Technology

**Additive Manufacturing of PLA-based Composites Using a Colloidal Feedstock: Biodegradable and Permanent Scaffolds in Medical Applications:** *Begoña Ferrari*<sup>1</sup>; Ana Ferrandez-Montero<sup>1</sup>; Alvaro Eguiluz<sup>2</sup>;

*Antonio Javier Sanchez-Herencia*<sup>1</sup>; <sup>1</sup>Instituto de Cerámica y Vidrio, CSIC

**Enzymes Immobilized on Nanocarriers for the Degradation of Synthetic Polymers:** *Eva Krakor*<sup>1</sup>; Sanjay Mathur<sup>1</sup>; Isabel Gessner<sup>1</sup>;

Michael Wilhelm<sup>1</sup>; <sup>1</sup>University of Cologne

**Impact of Wall Thickness and Pores Size Variation on Hydroxyapatite Based Triply Periodic Minimal Surfaces:** *Islam Bouakaz*<sup>1</sup>; David Grossin<sup>2</sup>;

Gregory Nolens<sup>1</sup>; <sup>1</sup>CERHUM; <sup>2</sup>Institut National Polytechnique de Toulouse

**4D Bioprinting for Making Hierarchical Composite Scaffolds for Blood Vessel Regeneration:** *Shangsi Chen*<sup>1</sup>; *Min Wang*<sup>1</sup>;

<sup>1</sup>University of Hong Kong

**Light-adaptive Dynamic DNA-based Hydrogel:** *Joonas Ryssy*<sup>1</sup>; Sessa Manuguri<sup>1</sup>; Anton Kuzyk<sup>1</sup>;

<sup>1</sup>Aalto University

## BIOMATERIALS

### Next Generation Biomaterials — On-Demand Poster Presentations

**Sponsored by:** ACerS Bioceramics Division, TMS Biomaterials Committee

**Program Organizers:** Roger Narayan, University of North Carolina; Min Wang, University of Hong Kong; Shawn Allan, Lithoz America LLC

Friday AM | October 22, 2021

On-Demand Poster Hall | MS&T On Demand

**4D Printed Shape Morphing PDLLA-co-TMC/GelMA Scaffolds for Tissue Regeneration:** *Xiaodie Chen*<sup>1</sup>; *Jiahui Lai*<sup>1</sup>; *Min Wang*<sup>1</sup>;

<sup>1</sup>University of Hong Kong

**Metal Release from a Biomedical CoCrMo Alloy in Mixed Protein Solutions under Static and Sliding Conditions – Effects of Protein Aggregation and Metal Precipitation:** *Zheng Wei*<sup>1</sup>;

Valentin Romanovski<sup>2</sup>; Luimar Filho<sup>3</sup>; Cecilia Cecilia<sup>3</sup>; Yolanda Hedberg<sup>1</sup>;

<sup>1</sup>Western University; <sup>2</sup>National Academy of Sciences of Belarus;

<sup>3</sup>Uppsala University

## FUNDAMENTALS AND CHARACTERIZATION

### Nucleation of Solid-State Phase Transformations — On-Demand Oral Presentations

**Sponsored by:** TMS Phase Transformations Committee

**Program Organizers:** Eric Lass, University of Tennessee-Knoxville; Sophie Primig, University of New South Wales; Keith Knipling, Naval Research Laboratory

Friday AM | October 22, 2021

On-Demand Room 7 | MS&T On Demand

**Effect of Cooling Rate and Austenitic Grain Size on the Austenite Decomposition Kinetics in a Low-carbon Steel:** *Carlos Alberto Barajas-Miguel*<sup>1</sup>;

Octavio Vázquez-Gómez<sup>2</sup>; *Antonio Oliver-Reynoso*<sup>1</sup>; Edgar López-Martínez<sup>2</sup>; Héctor Javier Vergara-Hernández<sup>1</sup>;

<sup>1</sup>Tecnológico Nacional de México/I.T. Morelia; <sup>2</sup>Universidad del Istmo

**3-dimensional Observation of Bainite from Austenite Grain Boundary in 0.6wt% Carbon Steel:** *Shotaro Jimbo*<sup>1</sup>; Shoichi Nambu<sup>1</sup>;

<sup>1</sup>University of Tokyo

**Identification of Critical Nucleation Events by the Gromov-Wasserstein Distance:** *Jeremy Mason*<sup>1</sup>; Sakura Kawano<sup>1</sup>;

<sup>1</sup>University of California, Davis

## SPECIAL TOPICS

### Online Teaching Best Practices for the COVID Era and Beyond — On-Demand Oral Presentations

**Sponsored by:** ACerS Electronic Division

**Program Organizers:** B. Reeya Jayan, Carnegie Mellon University; Jennifer Andrew, University of Florida

Friday AM | October 22, 2021

On-Demand Room 13 | MS&T On Demand

**Session Chair:** B. Reeya Jayan, Carnegie Mellon University

## Invited

**Debunking the Hidden Curriculum in Online STEM Courses: A Depiction of Three Latinx Engineering Educators:** *Idalis Villanueva-Alarcón*<sup>1</sup>;

John Mendoza-García<sup>1</sup>; Sinda Rivera-Jiménez<sup>1</sup>;

<sup>1</sup>University of Florida

**Photonics Workforce Training Using Game-based Learning and Interactive Desktop Simulations:** *Erik Verlage*<sup>1</sup>;

<sup>1</sup>Massachusetts Institute of Technology

**Virtual Learning in Minecraft: Using a Game to Teach Materials Engineering:** *B. Reesha Jayan<sup>1</sup>; Chad Herschick<sup>1</sup>; Michael Melville<sup>1</sup>;*  
<sup>1</sup>Carnegie Mellon University

**Invited**

**Working Together Apart: Design Thinking and Sustainable Engineering Design Projects Online:** *Nancy Ruzyski<sup>1</sup>;* <sup>1</sup>University of Florida

## CERAMIC AND GLASS MATERIALS

### Phase Transformations in Ceramics: Science and Applications — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Scott McCormack, University of California, Davis; Pankaj Sarin, Oklahoma State University; Sanjay V. Khare, University of Toledo; Waltraud Kriven, University of Illinois at Urbana-Champaign

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

**Invited**

**New Insight into the Disorder Mechanism in Fluorite-related Ceramics:** *Maik Lang<sup>1</sup>;* <sup>1</sup>University of Tennessee

**Invited**

**Phase Stability and Transformation in Borides Examined by X-ray Diffraction:** *James Cahill<sup>1</sup>;* <sup>1</sup>Lawrence Livermore National Laboratory

**Invited**

**Prediction of Diffusion-less Phase Transformations:** *Randall Hay<sup>1</sup>;* Emmanuel Boakye<sup>2</sup>; Pavel Mogilevsky<sup>1</sup>; Thomas Key<sup>1</sup>; <sup>1</sup>U.S. Air Force Research Laboratory

**Order-disorder Relationships in Zirconium Carbides:** *Theresa Davey<sup>1</sup>;* Ying Chen<sup>1</sup>; <sup>1</sup>Tohoku University

**Computation of Fracture, Twinning, and Amorphization in Anisotropic Single and Polycrystalline Real-structured B4C Using Phase Field Approaches in the Finite Element Method:** *Benhour Amirian<sup>1</sup>;* Bilen Abali<sup>2</sup>; Mali Moshtaghoun<sup>3</sup>; Jonathan Ligda<sup>4</sup>; Debjoy Mallick<sup>5</sup>; James Hogan<sup>1</sup>; <sup>1</sup>University of Alberta; <sup>2</sup>Technische Universität Berlin; <sup>3</sup>Spanish Ministry of Science and Innovation; <sup>4</sup>DEVCOM Army Research Laboratory; <sup>5</sup>Amy Research Laboratory

## MODELING

### Phonon Properties of Materials: Modeling and Experimentation — On-Demand Oral Presentations

**Sponsored by:** TMS Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Conversion and Storage Committee

**Program Organizers:** Murali Gopal Muraleedharan, Oak Ridge National Laboratory; Zhe Cheng, University of Illinois at Urbana-Champaign; Kiarash Gordiz, Massachusetts Institute of Technology

**Friday AM | October 22, 2021**  
**On-Demand Room 10 | MS&T On Demand**

**Invited**

**Phonons and Twisting Symmetries in Non-symorphic Materials:** *Lucas Lindsay<sup>1</sup>;* <sup>1</sup>Oak Ridge National Laboratory

**Invited**

**Transfer Learning for Phonon and Thermal Property Predictions:** *Zeyu Liu<sup>1</sup>;* *Tengfei Luo<sup>1</sup>;* <sup>1</sup>University of Notre Dame

**Invited**

**High-temperature Heat Transport in Anharmonic Systems at the Nanoscale:** *Keivan Esfarjani<sup>1</sup>;* <sup>1</sup>University of Virginia

**Experimental and Computational Thermal Conductivity Reduction in Single Crystal Thorium Dioxide from Lattice Defects:** *Cody Dennett<sup>1</sup>;* Marat Khafizov<sup>2</sup>; Anter El-Azab<sup>3</sup>; David Hurley<sup>1</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>Ohio State University; <sup>3</sup>Purdue University

**Tailoring Thermal Transport in Insulators Using Energetic Ions:** *Vinay Chauhan<sup>1</sup>;* Joshua Ferrigno<sup>1</sup>; Saqeeb Adnan<sup>1</sup>; Zhandos Utegulov<sup>2</sup>; Cody Dennett<sup>3</sup>; Amey Khanolkar<sup>3</sup>; Zilong Hua<sup>3</sup>; Lingfeng He<sup>3</sup>; David Hurley<sup>3</sup>; *Marat Khafizov<sup>1</sup>;* <sup>1</sup>Ohio State University; <sup>2</sup>Nazarbayev University; <sup>3</sup>Idaho National Laboratory

**Understanding Ionic Conduction Mechanisms in Glassy Electrolytes Using MD Vibrational Analysis:** *Cameron Beg<sup>1</sup>;* John Kieffer<sup>1</sup>; <sup>1</sup>University of Michigan

## BIOMATERIALS

### Porous Materials for Biomedical Applications — On-Demand Oral Presentations

**Sponsored by:** ACerS Bioceramics Division

**Program Organizers:** Usman Liaqat, National University of Sciences and Technology; Chuanbin Mao, University of Oklahoma; Mingying Yang, Zhejiang University

**Friday AM | October 22, 2021**  
**On-Demand Room 3 | MS&T On Demand**

**Corrosion of Mechanically Milled, Annealed, and Biocompatible Magnesium Alloys for Osteopathic Tissue Regeneration:** *Adam Rutherford<sup>1</sup>;* Mark Atwater<sup>1</sup>; Julian Tse Lop Kun<sup>1</sup>; <sup>1</sup>Liberty University

# Technical Program

## PROCESSING AND MANUFACTURING

### Powder Metallurgical Components in High Performance Applications — On-Demand Oral Presentations

**Sponsored by:** TMS Powder Materials Committee

**Program Organizers:** Peng Cao, The University of Auckland; Hanadi Salem, American University in Cairo; Paul Prichard, Kennametal Inc.; Matthew Osborne, Global Advanced Metals; James Paramore, US Army Research Laboratory

**Friday AM | October 22, 2021**  
**On-Demand Room 12 | MS&T On Demand**

**Session Chair:** Peng Cao, University of Auckland

**Cemented Carbides with Complex Binder Alloys:** *Yong Liu<sup>1</sup>*; <sup>1</sup>Central South University

**Development of Eco-friendly POM Binder System for High Strength Ti-MIM:** *Keemi Lim<sup>1</sup>*; Muhammad Hayat<sup>1</sup>; Peng Cao<sup>1</sup>; <sup>1</sup>The University of Auckland

**Fabrication of Titanium and Titanium Alloy Components by Thermomechanical Powder Consolidation:** *Deliang Zhang<sup>1</sup>*; <sup>1</sup>Northeastern University

**High-strength Titanium Matrix Composites Reinforced with In Situ Polycarbosilane-derived TiC Particle:** *Xin Lu<sup>1</sup>*; Yu Pan<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

**Microstructural Uniformity during Sintering, Thermal-plastic Processing and Recrystallization of Tungsten:** *Lin Zhang<sup>1</sup>*; Xingyu Li<sup>1</sup>; Xuanhui Qu<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

**Thermodynamic Model for Predicting the Embodied Energy of Titanium Alloys Produced by Powder Metallurgy:** *James Paramore<sup>1</sup>*; Brady Butler<sup>1</sup>; Matthew Dunstan<sup>1</sup>; <sup>1</sup>US Army Research Laboratory

**Synthesis of Low-oxygen Titanium towards Achieving Strength-ductility Synergy:** *Kumar Jena<sup>1</sup>*; Ying Xu<sup>1</sup>; Peng Cao<sup>1</sup>; <sup>1</sup>University Of Auckland

**Synthesis, Sintering and Mechanical Behavior of Ultra-fine Low-oxygen Titanium Powder:** *Ying Xu<sup>1</sup>*; Kumar Jena<sup>1</sup>; Peng Cao<sup>1</sup>; <sup>1</sup>The University of Auckland

**Effect of Manufacturing Parameters on Inoculated PM Tool Steel Properties:** Randa Habib<sup>1</sup>; Ayman Elsayed<sup>1</sup>; Saiid Anwar<sup>1</sup>; Bahaa Salah<sup>1</sup>; Taha Mattar<sup>1</sup>; <sup>1</sup>Central Metallurgical Research and Development Institute

**Selective Laser Melting of Metallic Glass Powder to Improve Chemical and Mechanical Performance of Magnesium:** *Xiyu Yao<sup>1</sup>*; <sup>1</sup>Southern University of Science and Technology

## CERAMIC AND GLASS MATERIALS

### Preceramic Polymers; Synthesis, Processing, Modeling, and Derived Ceramics — On-Demand Oral Session: Preceramic Polymers

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Matthew Dickerson, Air Force Research Laboratory; Gurpreet Singh, Kansas State University; Paolo Colombo, University of Padova; Günter Motz, Universität Bayreuth

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

**Session Chair:** Matthew Dickerson, Air Force Research Laboratory

#### Invited

**Novel Hydrogen Chemisorption Properties of Polymer-derived Amorphous SiAlN Compounds:** *Yuji Iwamoto<sup>1</sup>*; <sup>1</sup>Nagoya Institute of Technology

#### Invited

**Synthesis and 3D Printing of Antibacterial Polymer-derived Bioceramic Scaffolds for Bone Engineering Applications:** Joelle El Hayek<sup>1</sup>; Laurence Soussan<sup>1</sup>; Philippe Miele<sup>1</sup>; Mikhael Bechelany<sup>1</sup>; *Chrystelle Salameh<sup>1</sup>*; <sup>1</sup>Institut Européen des Membranes

#### Invited

**Polymer-derived UHTC Synthesis:** *Matthew Laskoski<sup>1</sup>*; <sup>1</sup>US Naval Research Lab

**Superparamagnetic Silicon Carbonitride Ceramic Fibers through In-situ Generation of Iron Silicide Nanoparticles:** *Günter Motz<sup>1</sup>*; Antoine Viard<sup>1</sup>; Birgit Weber<sup>1</sup>; Samuel Bernard<sup>2</sup>; <sup>1</sup>University of Bayreuth; <sup>2</sup>CNRS IRCER Limoges

**Thermomechanical Performance of a Novel Class of Ultra-high Temperature Polymer Derived La Containing Zr-B-C-(O) Ceramics:** *Gokul Gopakumar<sup>1</sup>*; Ganesh T<sup>1</sup>; Renjith Devasia<sup>2</sup>; Ravi Kumar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Madras; <sup>2</sup>Vikram Sarabhai Space Centre

**Laser and Furnace Pyrolyzed Organosilazane-based Glass/ZrO<sub>2</sub> Composite Coating Systems: A Comparison:** *Alexander Horcher<sup>1</sup>*; Katja Tangermann-Gerk<sup>2</sup>; Walter Krenkel<sup>1</sup>; Günter Motz<sup>1</sup>; <sup>1</sup>University of Bayreuth; <sup>2</sup>Bayerisches Laserzentrum Erlangen

**Additive Manufacturing of Hybrid Polymer-derived Ceramics via Core-shell Direct-ink Writing:** *Robert Pack<sup>1</sup>*; James Kemp<sup>1</sup>; Brett Compton<sup>1</sup>; <sup>1</sup>University of Tennessee Knoxville

**Metal-coordinated Preceramic Polymer Hairy Nanoparticles for Ultra-high Temperature Structural Materials:** *Maria Parvulescu<sup>1</sup>*; Kara Martin<sup>2</sup>; Christina Thompson<sup>2</sup>; Matthew Dickerson<sup>2</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>AFRL

**SiOC Coatings on Yttria Stabilized Zirconia Microspheres Using a Fluidized Bed Coating Process:** Sanjay Kumar<sup>1</sup>; *Kathy Lu<sup>1</sup>*; <sup>1</sup>Virginia Polytechnic Institute and State University

**Preceramic Polymer Organization via Block Copolymer Templating:**

*John Bowen*<sup>1</sup>; Lisa Rueschhoff<sup>2</sup>; Shahryar Mooraj<sup>3</sup>; Jacob Goodman<sup>4</sup>; Emily Davidson<sup>5</sup>; Benito Roman-Manso<sup>6</sup>; K. L. Martin<sup>1</sup>; Scott Schiffres<sup>4</sup>; Wen Chen<sup>3</sup>; Matthew Dickerson<sup>2</sup>; Jennifer Lewis<sup>5</sup>; <sup>1</sup>UES Inc.; <sup>2</sup>Air Force Research Lab; <sup>3</sup>University of Massachusetts Amherst; <sup>4</sup>Binghamton University; <sup>5</sup>Harvard University

**Isoconversional Methods and Kinetic Reaction Models for Cure Modelling of Commercial Pre-ceramic Polymers and their Blends:**

*Zlatomir Apostolov*<sup>1</sup>; Elizabeth Heckman<sup>2</sup>; Michael Cinibulk<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>Wright State University

**Impact of Preceramic Polymer Architecture on Derived Ceramics:**

*Timothy Pruyne*<sup>1</sup>; Matthew Dickerson<sup>1</sup>; Brandon Ackley<sup>1</sup>; <sup>1</sup>Materials and Manufacturing Directorate

**Evolutive State and Damage Modeling and Characterization for PIP-based Hypersonic Vehicle Materials:**

*Rick Hall*<sup>1</sup>; Zlatomir Apostolov<sup>1</sup>; Ashley Hilmas<sup>1</sup>; George Jefferson<sup>1</sup>; Vikas Varshney<sup>1</sup>; Michael Cinibulk<sup>1</sup>; Robert Brockman<sup>2</sup>; Rebecca Hoffman<sup>2</sup>; Thomas Key<sup>3</sup>; Derek King<sup>3</sup>; <sup>1</sup>Air Force Research Laboratory; <sup>2</sup>University of Dayton Research Institute; <sup>3</sup>UES

**Embedded Direct Ink Writing of Freeform Ceramic Components:**

*Kai Huang*<sup>1</sup>; Hamada Elsayed<sup>1</sup>; Giorgia Franchin<sup>1</sup>; Paolo Colombo<sup>1</sup>; <sup>1</sup>University of Padova

**Study on Manufacturing of Silsesquiazane Derived Hierarchically Porous Silicon Carbonitride Ceramics with Aligned Macropore by Freeze-casting Method:**

*Tae-Hwan Huh*<sup>1</sup>; Young-Je Kwark<sup>1</sup>; <sup>1</sup>Soongsil University

**CERAMIC AND GLASS MATERIALS**

**Preceramic Polymers; Synthesis, Processing, Modeling, and Derived Ceramics – On-Demand Poster Presentations**

**Sponsored by:** ACerS Engineering Ceramics Division

**Program Organizers:** Matthew Dickerson, Air Force Research Laboratory; Gurpreet Singh, Kansas State University; Paolo Colombo, University of Padova; Günter Motz, Universität Bayreuth

**Friday AM | October 22, 2021**

**On-Demand Poster Hall | MS&T On Demand**

**Session Chair:** Joe Bowen, Air Force Research Laboratory

**Fabrication of SiOC Fibermats via Electrospinning and their Applications in Energy Storage Systems:** *Shakir Bin Mujib*<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University

**Investigation of Polymer Derived SiOC/Carbon Nanotube Electrodes for Na-ion Batteries:** *Mabel Anstine*<sup>1</sup>; Shakir Bin Mujib<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University

**Porous SiOC/SiC Ceramics via an Active-filler Catalyzed Polymer-derived Method:** *Advaith Rau*<sup>1</sup>; Kathy Lu<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University

**Synthesis of Precursor Derived Si(B)CN Ceramic Coating for High-temperature Applications:** *Lanie Mannebach*<sup>1</sup>; Shakir Bin Mujib<sup>1</sup>; Gurpreet Singh<sup>1</sup>; <sup>1</sup>Kansas State University

**FUNDAMENTALS AND CHARACTERIZATION**

**Probing Defect Properties and Behavior under Mechanical Deformation and Extreme Conditions – On-Demand Oral Session: Defect Property, Characterization, and Evolution**

**Sponsored by:** TMS Nanomechanical Materials Behavior Committee, TMS Nuclear Materials Committee, TMS Mechanical Behavior of Materials Committee

**Program Organizers:** Zhe Fan, Lamar University; Tianyi Chen, Oregon State University; Shijun Zhao, City University of Hong Kong; Mitra Taheri, Johns Hopkins University; Yury Osetskiy, Oak Ridge National Laboratory

**Friday AM | October 22, 2021**

**On-Demand Room 7 | MS&T On Demand**

**Invited**

**Defect Absorption at Grain Boundaries: A Grain Boundary Structure Perspective:** *David Srolovitz*<sup>1</sup>; Jian Han<sup>1</sup>; Larissa Woryk<sup>2</sup>; Mitra Taheri<sup>3</sup>; Jaime Marian<sup>4</sup>; <sup>1</sup>City University of Hong Kong; <sup>2</sup>University of Pennsylvania; <sup>3</sup>Johns Hopkins University; <sup>4</sup>University of California, Los Angeles

**Invited**

**Automated Defect Detection in Electron Microscopy with Machine Learning:** *Dane Morgan*<sup>1</sup>; Ryan Jacobs<sup>1</sup>; Mingren Shen<sup>1</sup>; Kevin Field<sup>2</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>University of Michigan

**Invited**

**Effects of Cr On 1/2<111> to <100> Loop Transformation in Concentrated Fe-Cr Alloys under Irradiation:** *Xian-Ming Bai*<sup>1</sup>; <sup>1</sup>Virginia Polytechnic Institute and State University

**Invited**

**A Statistical Approach for Atomistic Calculations of Vacancy Formation Energy and Chemical Potentials in Concentrated Solid-solution Alloys:** *Yongfeng Zhang*<sup>1</sup>; Anus Manzoor<sup>2</sup>; Chao Jiang<sup>3</sup>; Dilpuneet Aidhy<sup>2</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>University of Wyoming; <sup>3</sup>Idaho National Laboratory

**Defect Properties and Deformation Mechanisms of Multi-component Intermetallics:** *Shijun Zhao*<sup>1</sup>; <sup>1</sup>City University of Hong Kong

**Invited**

**Irradiation-induced Self-organization of the Microstructure in Irradiated Alloys and Its Influence on Mechanical Properties:** *Pascal Bellon*<sup>1</sup>; Qun Li<sup>1</sup>; Gabriel Bouobda Moladje<sup>1</sup>; Sung-Eun Kim<sup>1</sup>; Soumyajit Jana<sup>1</sup>; Robert Averback<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign



# Technical Program

## Invited

**Machine Learning Driven In-situ TEM with Ion Irradiation:** *Meimei Li*<sup>1</sup>;  
<sup>1</sup>Argonne National Laboratory

## Invited

**Lattice Distortion in NbTaTiV and NbTaTiVZr Refractory High-entropy Alloys:** Chanho Lee<sup>1</sup>; Yi Chou<sup>2</sup>; George Kim<sup>3</sup>; Michael Gao<sup>4</sup>; Ke An<sup>5</sup>; Jamieson Brecht<sup>1</sup>; Chuan Zhang<sup>6</sup>; Wei Chen<sup>3</sup>; Jonathan Poplawsky<sup>5</sup>; Gian Song<sup>7</sup>; Yi-Chia Chou<sup>2</sup>; *Peter Liaw*<sup>8</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>National Chiao Tung University; <sup>3</sup>Illinois Institute of Technology; <sup>4</sup>National Energy Technology Laboratory/Leidos Research Support Team; <sup>5</sup>Oak Ridge National Laboratory; <sup>6</sup>Computherm LLC; <sup>7</sup>Kongju National University; <sup>8</sup>University of Tennessee

## Invited

**Synchrotron High-energy X-ray Studies of Nuclear Structural Materials: Deformation and Additive Manufacturing:** *Xuan Zhang*<sup>1</sup>; Meimei Li<sup>1</sup>; Jonathan Almer<sup>1</sup>; Jun-Sang Park<sup>1</sup>; Peter Kenesei<sup>1</sup>; Andrew Chuang<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

## Invited

**The Role of Interfaces in Mechanical Response and Radiation Resistance of Ceramics:** *Izabela Szlufarska*<sup>1</sup>; Hongliang Zhang<sup>1</sup>; Jianqi Xi<sup>1</sup>; Xing Wang<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

## Invited

**Irradiation Defects and Strain-induced Martensitic Transformations:** *Janelle Wharry*<sup>1</sup>; Chao Yang<sup>1</sup>; Yangyang Zhao<sup>1</sup>; Keyou Mao<sup>2</sup>; Yash Pachaury<sup>1</sup>; Anter El-Azab<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Oak Ridge National Laboratory

## Invited

**Effects of Electronic Structures on Defect and Mechanical Properties of BCC Multicomponent Alloys:** Yong-Jie Hu<sup>1</sup>; *Liang Qi*<sup>2</sup>; <sup>1</sup>Drexel university; <sup>2</sup>University of Michigan

## Invited

**The Impact of Elastic Anisotropy on Hydride Morphology in Zirconium:** Pierre-Clement Simon<sup>1</sup>; *Michael Tonks*<sup>2</sup>; Arthur Motta<sup>1</sup>; Long-Qing Chen<sup>1</sup>; Mark Daymond<sup>3</sup>; <sup>1</sup>Pennsylvania State University; <sup>2</sup>University of Florida; <sup>3</sup>Queen's University

## Invited

**Impact of Carbon Nanotube Defects on Fracture Mechanisms in Ceramic Nanocomposites:** *Yingchao Yang*<sup>1</sup>; Brian Sheldon<sup>2</sup>; Izabela Szlufarska<sup>3</sup>; Jun Lou<sup>4</sup>; <sup>1</sup>University of Maine; <sup>2</sup>Brown University; <sup>3</sup>University of Wisconsin; <sup>4</sup>Rice University

## Invited

**Studying Radiation Effects in Nuclear Fuels via Advanced Characterization and Modeling:** *Lingfeng He*<sup>1</sup>; Kaustubh Bawane<sup>1</sup>; Tiankai Yao<sup>1</sup>; Pengyuan Xiu<sup>1</sup>; Marat Khafizov<sup>2</sup>; Miaomiao Jin<sup>3</sup>; Chao Jiang<sup>1</sup>; Cody Dennett<sup>1</sup>; Zilong Hua<sup>1</sup>; Anter El-Azab<sup>4</sup>; David Hurley<sup>1</sup>; Jian Gan<sup>1</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>The Ohio State University; <sup>3</sup>Pennsylvania State University; <sup>4</sup>Purdue University

## Invited

**Irradiation Response of FCC and BCC Compositionally Complex Alloys Using In-situ and Ex-situ Irradiations:** *Adrien Couet*<sup>1</sup>; Calvin Parkin<sup>1</sup>; Michael Moorehead<sup>1</sup>; Lin Shao<sup>2</sup>; Frank Garner<sup>1</sup>; Lingfeng He<sup>3</sup>; Pengyuan Xiu<sup>3</sup>; Wei-Ying Chen<sup>4</sup>; Meimei Li<sup>4</sup>; Kumar Sridharan<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>Texas A&M University; <sup>3</sup>Idaho National Laboratory; <sup>4</sup>Argonne National Laboratory

**Effects of Annealing and Ion Irradiation on Helium Implanted NiCo and NiFe Concentrated Solid-solution Alloys:** *Zhe Fan*<sup>1</sup>; Xing Wang<sup>1</sup>; Di Chen<sup>2</sup>; Yongqiang Wang<sup>2</sup>; Yuri Osetsky<sup>1</sup>; Hongbin Bei<sup>1</sup>; William Weber<sup>3</sup>; Yanwen Zhang<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>The University of Tennessee

**Deformation Microstructure of Ferritic/Martensitic Steels after Spallation Neutron Irradiation:** *Kun Wang*<sup>1</sup>; <sup>1</sup>Alfred University

**Elemental Partitioning Behavior among Precipitates in Alumina-forming-austenitic Stainless Steel:** *Qing-Qiang Ren*<sup>1</sup>; David Hoelzer<sup>1</sup>; Michael Lance<sup>1</sup>; Yukinori Yamamoto<sup>1</sup>; Michael Brady<sup>1</sup>; Jonathan Poplawsky<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

**Survey of Defect Absorption Effects in Grain Boundaries:** *Larissa Woryk*<sup>1</sup>; David Srolovitz<sup>2</sup>; Jian Han<sup>2</sup>; <sup>1</sup>University of Pennsylvania; <sup>2</sup>City University of Hong Kong

**Enhanced Load Transfer and Ductility in Al-9Ce Alloy through Heterogeneous Lamellar Microstructure Design by Cold Rolling and Annealing:** *Chi Zhang*<sup>1</sup>; <sup>1</sup>Shanghai Jiao Tong University

**Influence of Microstructural Variation on Spall Failure of Al7085:** *Dung-Yi Wu*<sup>1</sup>; Chengyun Miao<sup>1</sup>; Christopher DiMarco<sup>1</sup>; K.T. Ramesh<sup>1</sup>; Todd C. Hufnagel<sup>1</sup>; <sup>1</sup>Johns Hopkins University

**Switching the Fracture Toughness of Single Crystal ZnS by Light Irradiation:** Tingting Zhu<sup>1</sup>; Kuan Ding<sup>1</sup>; Anahid Amiri<sup>1</sup>; Yu Oshima<sup>2</sup>; Enrico Bruder<sup>1</sup>; Robert Stark<sup>1</sup>; Karsten Durst<sup>1</sup>; Katsuyuki Matsunaga<sup>2</sup>; Atsutomu Nakamura<sup>2</sup>; *Xufei Fang*<sup>1</sup>; <sup>1</sup>Technische Universität Darmstadt; <sup>2</sup>Nagoya University

## FUNDAMENTALS AND CHARACTERIZATION

### Processing—Microstructure—Property Relationships of Titanium and Titanium Alloys — On-Demand Oral Presentations

**Sponsored by:** TMS Titanium Committee

**Program Organizers:** Yufeng Zheng, University of Nevada-Reno; Rongpei Shi, Lawrence Livermore National Laboratory; Michael Gram, Titanium Metals Corporation

**Friday AM | October 22, 2021**  
**On-Demand Room 7 | MS&T On Demand**

**Deformation Behavior of Ti-Ni-Fe Based Ternary B2 Pseudo Binary Intermetallic:** *Subha Panda*<sup>1</sup>; Jayant Jain<sup>2</sup>; Sudhanshu Singh<sup>3</sup>; <sup>1</sup>Indian Institute of Technology Kanpur; <sup>2</sup>IIT Delhi; <sup>3</sup>IIT Kanpur

## PROCESSING AND MANUFACTURING

### Processing and Performance of Materials Using Microwaves, Electric and Magnetic Fields, Ultrasound, Lasers, and Mechanical Work: The Rustum Roy Symposium — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Manufacturing Division

**Program Organizers:** Morsi Mahmoud, King Fahd University of Petroleum & Minerals; Dinesh Agrawal, Pennsylvania State University; Guido Link, Karlsruhe Institute of Technology; Motoyasu Sato, Chubu University; Rishi Raj, University of Colorado; Christina Wildfire, National Energy Technology Laboratory; Zhiwei Peng, Central South University

**Friday AM | October 22, 2021**  
**On-Demand Room 12 | MS&T On Demand**

#### Invited

**Characterizing the Kinetics of Isothermal Microwave-assisted Chemical Syntheses (IMACS): Application of a Unified Process Kinetic Equation (UPKE):** *Boon Wong*<sup>1</sup>; <sup>1</sup>Retired

#### Invited

**Micro Flash Sintering for Additive Manufacturing of Ceramics:** *Rubens Ingraci Neto*<sup>1</sup>; Rishi Raj<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>University of Colorado

#### Invited

**Conditions for the Microwave Effect:** Motoyasu Sato<sup>1</sup>; *Shin Nakatani*<sup>1</sup>; <sup>1</sup>Chubu University

**Novel Electrode Configuration Effects on the Microstructural Homogeneity of Flash Sintered Ceramics for Solid-state Battery Electrolytes:** *Gareth Jones*<sup>1</sup>; Chris Green<sup>2</sup>; Sherry Ghanizadeh<sup>2</sup>; David Pearmain<sup>2</sup>; Geoff West<sup>1</sup>; Emma Kendrick<sup>3</sup>; Claire Dancer<sup>1</sup>; <sup>1</sup>University of Warwick; <sup>2</sup>Lucideon Ltd; <sup>3</sup>University of Birmingham

**Methodology for Scaling Microwave Catalyst in a Fixed Bed:** *Christina Wildfire*<sup>1</sup>; Yan Zhou<sup>1</sup>; Christopher Marin<sup>1</sup>; Doug Kauffman<sup>1</sup>; Dushyant Shekawat<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

## MATERIALS-ENVIRONMENT INTERACTIONS

### Progressive Solutions to Improve Corrosion Resistance for Nuclear Waste Storage — On-Demand Alternative Nuclear Waste Storage Materials and New Imaging Neutron Microscopy Technique for Nuclear Waste Storage Glass Corroded in Aqueous Solution

**Sponsored by:** TMS Corrosion and Environmental Effects Committee, ACerS Glass & Optical Materials Division

**Program Organizers:** Madeleine Jordache, Stevens Institute of Technology; Gary Pickrell, Virginia Tech

**Friday AM | October 22, 2021**  
**On-Demand Room 9 | MS&T On Demand**

**Session Chairs:** Madeleine Jordache, Stevens Institute of Technology; Gary Pickrell, Virginia Tech

**Introductory Comments:** *Madeleine Jordache*<sup>1</sup>; <sup>1</sup>Stevens Institute of Technology

#### Invited

**Particulars of Crystallization of Glass-ceramics for Nuclear Waste Storage:** *Edgar Zanotto*<sup>1</sup>; <sup>1</sup>Federal University of Sao Carlos

#### Invited

**Neutron Microscope Based on Wolter Optics for Imaging Hydrogen Distribution in Glass:** *Boris Khaykovich*<sup>1</sup>; Daniel Hussey<sup>2</sup>; Suzanne Romaine<sup>3</sup>; Kiranmayee Kilaru<sup>4</sup>; Brian Ramsey<sup>4</sup>; <sup>1</sup>Massachusetts Institute of Technology; <sup>2</sup>NIST; <sup>3</sup>Harvard-Smithsonian Center for Astrophysics; <sup>4</sup>NASA

## CERAMIC AND GLASS MATERIALS

### Solid-state Optical Materials and Luminescence Properties — On-Demand Oral Presentations

**Sponsored by:** ACerS Basic Science Division, ACerS Engineering Ceramics Division, ACerS Glass & Optical Materials Division

**Program Organizers:** Yiquan Wu, Alfred University; Jas Sanghera, Naval Research Laboratory; Akio Ikesue, World-Lab. Co., Ltd; Rong-Jun Xie, Xiamen University; Mathieu Allix, University of Orleans; Kiyoshi Shimamura, National Institute for Materials Science; Liangbi Su, Shanghai Institute of Ceramics; Dariusz Hreniak, Institute of Low Temperature and Structure Research

**Friday AM | October 22, 2021**  
**On-Demand Room 4 | MS&T On Demand**

#### Invited

**Comonomer Isomers Result in LWIR-Transmitting ORMOCHALC Polymers:** *Darryl Boyd*<sup>1</sup>; Vinh Nguyen<sup>1</sup>; Frederic Kung<sup>2</sup>; Jason Myers<sup>1</sup>; Daniel Gibson<sup>1</sup>; Colin Baker<sup>1</sup>; Woohong Kim<sup>1</sup>; Jasbinder Sanghera<sup>1</sup>; <sup>1</sup>US Naval Research Laboratory; <sup>2</sup>University Research Foundation

# Technical Program

## Invited

**Enhancing Strength in Nanocrystalline Transparent Ceramics:** *Ricardo Castro*<sup>1</sup>; <sup>1</sup>University of California, Davis

## Invited

**A Green Chemistry Approach for the Preparation of Lanthanide Doped Alkaline-earth Fluoride Nanoparticles:** Chiara Cressoni<sup>1</sup>; Nicola Da Roit; Emil Milan<sup>1</sup>; Francesca Parolini<sup>2</sup>; Mariapina D'Onofrio<sup>2</sup>; Giacomo Lucchini<sup>1</sup>; *Adolfo Speghini*<sup>1</sup>; <sup>1</sup>University of Verona and INSTM; <sup>2</sup>University of Verona

## Invited

**Searching Nitride Luminescent Materials for Applications in High Luminance Lighting and Sensing:** *Rong-Jun Xie*<sup>1</sup>; <sup>1</sup>Xiamen University

## Invited

**Versatile Non-cubic Transparent Ceramics Applicable to Broad Wavelength Region:** Ho Jin Ma<sup>1</sup>; *Do-Kyung Kim*<sup>1</sup>; <sup>1</sup>Korea Advanced Institute of Science & Tech

**Micro- and Submicro-defects in Magneto-optical Crystal CeF<sub>3</sub>:** *Dongsheng Yuan*<sup>1</sup>; Encarnación G. Villora<sup>2</sup>; Kiyoshi Shimamura<sup>2</sup>; <sup>1</sup>National Institute for Materials Science; <sup>2</sup>NIMS

**Effect of Samarium Doping on the Phase Stability and Optical Properties of Agro-food Waste-derived Calcium Silicates:** *Manmeet Kaur*<sup>1</sup>; Kulvir Singh<sup>1</sup>; <sup>1</sup>SPMS, Thapar Institute of Engineering and Technology

## BIOMATERIALS

### Surface Engineering and Characterization of Titanium and Titanium Alloys – On-Demand Oral Sessions – Surface Engineering and Characterization of Titanium and Titanium Alloys

**Program Organizers:** Silvia Spriano, Politecnico di Torino; Yolanda Hedberg, KTH Royal Institute of Technology; James Noel, University of Western Ontario; Sara Ferraris, Politecnico Di Torino Disat; Fernando Warchomicka, Graz University of Technology

Friday AM | October 22, 2021

On-Demand Room 3 | MS&T On Demand

**Session Chairs:** Silvia Spriano, Politecnico di Torino - DISAT; Yolanda Hedberg, Western University, London, Ontario, Canada; James Noel, Western University, London, Canada; Sara Ferraris, Politecnico di Torino - DISAT; Fernando Warchomicka, Graz University of Technology

**Introductory Comments:** *Silvia Spriano*<sup>1</sup>; <sup>1</sup>Politecnico di Torino

**Effect of Various Reciprocating Geometries on Tribological Properties of SS 304 and Ti6Al4V under Dry and Lubricated Conditions:** *Chinmayee Nayak*<sup>1</sup>; Rishabh Kundu<sup>2</sup>; Rajneesh Pandey<sup>3</sup>; Kantesh Balani<sup>1</sup>; <sup>1</sup>Indian Institute of Technology, Kanpur; <sup>2</sup>National Institute of Technology, Rourkela; <sup>3</sup>Maulana Azad National Institute of Technology, Bhopal

**Observations on the Mechanically Assisted Crevice Corrosion of Titanium: Single Asperity Tribocorrosion of Titanium Alloy and Selective Dissolution of Beta Phase of Ti-6Al-4V in Physiologically Representative Conditions:** *Jeremy Gilbert*<sup>1</sup>; Annsley Mace<sup>1</sup>; Michael Kurtz<sup>2</sup>; Dongkai Zhu<sup>1</sup>; Yangping Liu<sup>1</sup>; <sup>1</sup>Clemson-MUSC Bioengineering Program

**Role of Patient Factors on Corrosion and Failure of Retrieved Metallic Artificial Hip and Knee Joint Implants:** *Saman Nikpour*<sup>1</sup>; Anastasia Codirenzi<sup>2</sup>; Matthew Teeter<sup>2</sup>; Yolanda Hedberg<sup>1</sup>; <sup>1</sup>Western University; <sup>2</sup>Western University Hospital

**Influence of Water Vapor on Metal and Oxygen Transport in Oxide Scale and Alpha-case Formation in Pure Titanium:** *Beyza Öztürk*<sup>1</sup>; Lukas Mengis<sup>1</sup>; Daniel Dickes<sup>2</sup>; Uwe Glatzel<sup>2</sup>; Mathias Galetz<sup>1</sup>; <sup>1</sup>DECHEMA Research Institute; <sup>2</sup>University of Bayreuth

**Electrophoretic Deposition, Microstructure and Properties of Multicomponent Sodium Alginate-based Coatings on Titanium Biomaterials:** *Tomasz Moskalewicz*<sup>1</sup>; Maciej Warcaba<sup>1</sup>; Marcin Kot<sup>1</sup>; Zoya Hadzhieva<sup>2</sup>; Aldo R. Boccaccini<sup>2</sup>; <sup>1</sup>AGH University of Science and Technology; <sup>2</sup>University of Erlangen-Nuremberg

**Growing Integration Layer [GIL] Strategy for Direct Formation of Bio-active Ceramic Coating on Metallic Alloy:** *Masahiro Yoshimura*<sup>1</sup>; Chi Huang Huang<sup>2</sup>; <sup>1</sup>National Cheng Kung University; Tokyo Institute of Technology; <sup>2</sup>National Cheng Kung University

**Plasma Electrolytic Oxidation of Titanium Alloys with Electron Beam Designed Topography:** Hugo Mora Sanchez<sup>1</sup>; Florian Pixner<sup>2</sup>; Ricardo Buzolin<sup>2</sup>; Raul Arrabal<sup>1</sup>; *Fernando Warchomicka*<sup>2</sup>; Endzhe Matykina<sup>1</sup>; <sup>1</sup>Universidad Complutense de Madrid; <sup>2</sup>Graz University of Technology

**Enhancing Differentiation of Preosteoblast on Selective Laser Melting Titanium Implants Treated with Mixed Acid and Heat:** *Phuc Le*<sup>1</sup>; Seine A. Shintani<sup>1</sup>; Hiroaki Takadama<sup>1</sup>; Morihiro Ito<sup>1</sup>; Tatsuya Kakutani<sup>1</sup>; Hisashi Kitagaki<sup>1</sup>; Shuntaro Terauchi<sup>1</sup>; Takaaki Ueno<sup>1</sup>; Hiroyuki Nakano<sup>1</sup>; Yoichiro Nakajima<sup>1</sup>; Kazuya Inoue<sup>1</sup>; Tomiharu Matsushita<sup>1</sup>; Seiji Yamaguchi<sup>1</sup>; <sup>1</sup>Chubu University

## PROCESSING AND MANUFACTURING

### Synthesis, Characterization, Modeling and Applications of Functional Porous Materials – On-Demand Oral Session: Functional Porous Materials

**Sponsored by:** ACerS Electronics Division, ACerS Engineering Ceramics Division

**Program Organizers:** Lan Li, Boise State University; Winnie Wong-Ng, National Institute of Standards and Technology; Kevin Huang, University of South Carolina

Friday AM | October 22, 2021

On-Demand Room 12 | MS&T On Demand

**Session Chair:** Lan Li, Boise State University

## Invited

**Probing the Mechanisms of Reactive Capture and Conversion of CO<sub>2</sub> into Inorganic Carbonates Using Architected Calcium and Magnesium Silicates:** Greeshma Gadikota<sup>1</sup>; Tianhe Yin<sup>1</sup>; Xun Gao<sup>1</sup>; *Hassnain Asgar*<sup>1</sup>; <sup>1</sup>Cornell University



**Invited**

**Hydrogen-bonded Organic Framework Materials for Gas Separation:** *Wei Zhou*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**Invited**

**Layer-by-layer Assembled Polymer/MOF Membrane for H<sub>2</sub>/CO<sub>2</sub> Separation:** *Fangming Xiang*<sup>1</sup>; David Hopkinson<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

**Invited**

**Small Molecules as Guests in Metal-organic Frameworks:** *Craig Brown*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**Invited**

**Thermodynamics of Molybdenum Oxide Clusters Encapsulated in Zeolite Y:** *Xianghui Zhang*<sup>1</sup>; Vitaliy Goncharov<sup>1</sup>; Cody Cockreham<sup>1</sup>; Esra Mertsoy<sup>1</sup>; Hui Sun<sup>2</sup>; Su Ha<sup>1</sup>; Jean-Sabin McEwen<sup>1</sup>; Xiaofeng Guo<sup>1</sup>; Di Wu<sup>1</sup>; <sup>1</sup>Washington State University; <sup>2</sup>East China University of Science and Technology

**Invited**

**Structure and CO<sub>2</sub> Adsorption Sites in the Flexible Coordination Polymer Ni-Dbm-Bpy from DFT:** *Eric Cockayne*<sup>1</sup>; Winnie Wong-Ng<sup>1</sup>; Andrew Allen<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**Invited**

**New Strategies for Defects Formation and Amorphization of Metal-organic Frameworks:** *Tomce Runcevski*<sup>1</sup>; <sup>1</sup>Southern Methodist University

**Material Characterization Testing of Synthetic Granular Composites Used in Equine Sports Surfaces:** *John Bridge*<sup>1</sup>; Charles Liu<sup>1</sup>; Elijah Leonen<sup>1</sup>; Kris Weissaupt<sup>2</sup>; Kaleb Dempsey<sup>3</sup>; <sup>1</sup>University of Washington; <sup>2</sup>MAP Laboratories LLC; <sup>3</sup>Racing Surfaces Testing Lab

**Chemical-aided Synthesis of Anorthite-sodalite-afghanite Porous Ceramics from Granite-clay-plantain Peel Mix:** *Odebole Oluwagbenga*<sup>1</sup>; Kashim Bolaji<sup>2</sup>; Akinbogun Lawrence<sup>1</sup>; Folorunso Oladayo<sup>1</sup>; <sup>1</sup>Federal University of Technology; <sup>2</sup>Federal University of Technology

**MATERIALS-ENVIRONMENT INTERACTIONS**

**Thermodynamics of Materials in Extreme Environments — On-Demand: Thermodynamics and Stabilities of Alloys and Ceramics**

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division

**Program Organizers:** Xiaofeng Guo, Washington State University; Kristina Lilova, Arizona State University; Kyle Brinkman, Clemson University; Alexandra Navrotsky, Arizona State University; Jake Amoroso, Savannah River National Laboratory; Xingbo Liu, West Virginia University; Gustavo Costa, NASA Glenn Research Center

**Friday AM | October 22, 2021**  
**On-Demand Room 9 | MS&T On Demand**

**Session Chairs:** Kristina Lilova, Arizona State University; Gustavo Costa, NASA Glenn Research Center

**Invited**

**Thermodynamics in the Design and Performance of Glass:** *Joseph Ryan*<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

**Invited**

**In-situ Hydrothermal Synthesis Calorimetry on Nonclassical Pathways of Nickel-aluminum Layered Double Hydroxide (NiAl-LDH) Formation:** *Xianghui Zhang*<sup>1</sup>; Cody Cockreham<sup>1</sup>; Esra Mertsoy<sup>1</sup>; Hui Sun<sup>2</sup>; Xiaofeng Guo<sup>1</sup>; Hongwu Xu<sup>3</sup>; Di Wu<sup>1</sup>; <sup>1</sup>Washington State University; <sup>2</sup>East China University of Science and Technology; <sup>3</sup>Los Alamos National Laboratory

**Strength, Deformation, and Equation of State of Tungsten Carbide to 66 GPa:** *Benjamin Brugman*<sup>1</sup>; Feng Lin<sup>2</sup>; Mingda Lv<sup>3</sup>; Curtis Kenney-Benson<sup>4</sup>; Dmitry Popov<sup>4</sup>; Lowell Miyagi<sup>2</sup>; Susannah Dorfman<sup>3</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>University of Utah; <sup>3</sup>Michigan State University; <sup>4</sup>HPCAT, Argonne National Lab

**Incorporation of Thorium and Uranium in the Monazite Structure by Wet Chemistry Route: Synthesis, Sintering and Long-term Behavior:** *Nicolas Dacheux*<sup>1</sup>; Danwen Qin<sup>2</sup>; Alison Roche<sup>1</sup>; Adel Mesbah<sup>3</sup>; Nicolas Clavier<sup>3</sup>; Stephanie Szenknect<sup>4</sup>; Renaud Podor<sup>3</sup>; <sup>1</sup>University of Montpellier; <sup>2</sup>ENSCM; <sup>3</sup>CNRS; <sup>4</sup>CEA

**Thermodynamic Properties of Special Alloys of the Ti-Al System Formed under SHS Conditions:** *Borys Sereda*<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Dmytro Kruglyak<sup>2</sup>; Yuriy Belokon<sup>2</sup>; <sup>1</sup>Dneprovsky State Technical University; <sup>2</sup>Zaporizhzhya National University

**Thermal and Microstructural Evolutions in Kerogen-rich Marcellus Shale:** *Cody Cockreham*<sup>1</sup>; Xianghui Zhang<sup>1</sup>; Miu Lun Lau<sup>2</sup>; Min Long<sup>2</sup>; Xiaofeng Guo<sup>1</sup>; Hongwu Xu<sup>3</sup>; Di Wu<sup>1</sup>; <sup>1</sup>Washington State University; <sup>2</sup>Boise State University; <sup>3</sup>Los Alamos National Laboratory

**High-temperature Structure and Thermodynamics of Cerium Silicates, A-Ce<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>, and Ce<sub>4.67</sub>(SiO<sub>4</sub>)<sub>3</sub>O:** *Andrew Strzelecki*<sup>1</sup>; Kyle Kriegsman<sup>2</sup>; Paul Estevenon<sup>3</sup>; Vitaliy Goncharov<sup>2</sup>; Jianming Bai<sup>4</sup>; Stephanie Szenknect<sup>3</sup>; Adel Mesbah<sup>3</sup>; Di Wu<sup>2</sup>; John McCloy<sup>5</sup>; Nicolas Dacheux<sup>3</sup>; Xiaofeng Guo<sup>2</sup>; <sup>1</sup>Washington State University; <sup>2</sup>Alexandra Navrotsky Institute for Experimental Thermodynamics, Washington State University; <sup>3</sup>ICSM, Univ Montpellier, CNRS, CEA, ENSCM, Site de Marcoule; <sup>4</sup>National Synchrotron Light Source II, Brookhaven National Laboratory; <sup>5</sup>Mechanical and Materials Engineering, Washington State University



# Technical Program

**Determination of the Activation Energy of the Formation of Intermetallic Compounds in the Ni-Al and Ti-Al System upon Receipt of Special Alloys:** Borys Sereda<sup>1</sup>; Dmytro Sereda<sup>1</sup>; Yuriy Belokon<sup>2</sup>; <sup>1</sup>Dneprovsky State Technical University; <sup>2</sup>Zaporizhzhya National University

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## MATERIALS-ENVIRONMENT INTERACTIONS

### Thermodynamics of Materials in Extreme Environments — On-Demand: Thermodynamics of Nuclear Materials and Minerals

**Sponsored by:** ACerS Basic Science Division, ACerS Energy Materials and Systems Division

**Program Organizers:** Xiaofeng Guo, Washington State University; Kristina Lilova, Arizona State University; Kyle Brinkman, Clemson University; Alexandra Navrotsky, Arizona State University; Jake Amoroso, Savannah River National Laboratory; Xingbo Liu, West Virginia University; Gustavo Costa, NASA Glenn Research Center

**Friday AM | October 22, 2021**  
**On-Demand Room 9 | MS&T On Demand**

**Session Chairs:** Xiaofeng Guo, Washington State University; Gustavo Costa, NASA Glenn Research Center

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#### Invited

**Thermodynamics of An-Cl Complexes at High Temperature and Pressure:** Ping Yang<sup>1</sup>; Xiaobin Zhang<sup>1</sup>; Morgan Kelley<sup>1</sup>; Jason Baker<sup>1</sup>; Hakim Boukhalfa<sup>1</sup>; Artaches Migdisov<sup>1</sup>; Hongwu Xu<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

#### Invited

**Dissolution of Uranium Based Dioxide in Nitric Acid: Impact of Fission Products and Microstructure:** Nicolas Dacheux<sup>1</sup>; Thomas Barral<sup>2</sup>; Thibault Kaczmarek<sup>2</sup>; Malvina Massonnet<sup>2</sup>; Laurent Claparede<sup>1</sup>; Nicolas Clavier<sup>3</sup>; Stephanie Szenknect<sup>2</sup>; Renaud Podor<sup>3</sup>; <sup>1</sup>University of Montpellier; <sup>2</sup>CEA; <sup>3</sup>CNRS

#### Invited

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