

TMS2021 VIRTUAL MARCH 15-18, 2021 • #TMSAnnualMeeting

www.tms.org/TMS2021

The content in this final program was generated on March 5, 2021. Please refer to the online session sheets for the most up-to-date information. *All times listed in this Final Technical Program are in EDT time zone (UTC-4:00).*

FINAL TECHNICAL PROGRAM



IMPORTANT

For full functionality of this mobilefriendly Technical Program PDF it is recommended that you have the Adobe Acrobat Reader™ app downloaded on your device:

- Open the App Store or the Google Play[™] Store and search "Adobe Acrobat Reader".
- Download the free PDF Reader application on your mobile device.

Open this PDF in Adobe Acrobat Reader and set the "View Settings" to "Continuous Pages".



ADOBE ACROBAT READER

The free global standard for reliably viewing PDFs.

It is recommended that you DO NOT PRINT this version of the Technical Program.



TABLE OF CONTENTS JUMP TO A DAY AND TIME.



MONDAY PM

TUESDAY AM

TUESDAY PM

WEDNESDAY AM

WEDNESDAY PM

THURSDAY AM

THURSDAY PM

POSTERS



MOBILE-FRIEND

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture in **Complex Alloys**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

Monday AM

March 15, 2021

Session Chair: David Bahr, Purdue University

8:30 AM

Introductory Comments: 100 Years and Still Cracking: A Griffith Fracture Symposium: Megan Cordill¹; ¹Erich Schmid Institute of Materials Science

8:35 AM Invited **Designing Ductility in BCC High Entropy Alloys?**: Eleanor Mak¹; Binglun Yin¹; *William* Curtin¹; ¹Epfl Sti Igm Lammm

9:15 AM

2,000 Years and Still Getting Dull: Mechanisms of Blade Chipping: Gianluca *Roscioli*¹; S. Mohadeseh Taheri-Mousavi¹; Cemal Tasan¹; ¹Massachusetts Institute of Technology

9:35 AM

A Length-scale Independent Phase-Field Model for Quantitative Prediction of **Ductile Fracture**: *William Huber*¹; Mohsen Asle Zaeem¹; ¹Colorado School of Mines

9:55 AM

Quantitative Phase-Field Modeling of Crack Propagation in Multi-Phase Material **Based on Griffith's Fracture Theory**: *Arezoo Emdadi*¹; Mohsen Asle Zaeem²; ¹Missouri University of Science and Technology; ²Colorado School of Mines

10:15 AM Invited **On the Fracture of Multi-element Metallic Alloys**: *Bernd Gludovatz*¹; Robert Ritchie²; ¹UNSW Sydney; ²Lawrence Berkeley National Laboratory

10:55 AM

On the Transition from Shear Banding to Fracture in Metals: In Situ Analysis of **Plastic Flow and Deformation Fields**: Shwetabh Yadav¹; Harshit Chawla¹; *Dinakar* Sagapuram¹; ¹Texas A&M University

11:15 AM

Probing Small-scale Fracture and Plasticity in Quasicrystals and High-entropy Alloys: Yu Zou¹; ¹University of Toronto

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Aluminum



Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Monday AM

March 15, 2021

Session Chair: Nima Shamsaei, Auburn University

8:30 AM Invited

Mechanical Behavior of Induced Lack of Fusion Flaws in AlSi10Mg: John *Lewandowski*¹; Brett Conner²; Austin Ngo¹; Varthula De Silva Jayasekera³; Griffin Jones⁴; Kenneth Meinert⁴; ¹Case Western Reserve University; ²DOE KC National Security Campus; ³Youngstown State University; ⁴Penn State University

9:00 AM

Cold Spray of Al and 6061 Al Alloy Powders: Effects of Oxide Thickness: Trevor *Bond*¹; Mobin Vandadi¹; Arvand Navabi¹; Vahid Rahneshin¹; Ridwan Ahmed¹; Nima Rahbar¹; Vic Champagne²; W.O. Soboyejo¹; ¹Worcester Polytechnic Institute; ²Army Research Laboratory

9:20 AM

Critical Fracture Toughness of Al 6061 Cold Spray Deposits: Scott Julien¹; Sinan Muftu¹; ¹Northeastern University



MOBILE-FRIEND

9:40 AM

Notch Sensitivity of AlSi10Mg Aluminum Alloy Produced by Laser Powder Bed Fusion Process: Avinesh Ojha; Wei-Jen Lai¹; Carlos Engler-Pinto¹; Xuming Su¹; ¹Ford Motor Company

10:00 AM Invited Interplay between Geometry, Defects, and Porosity on the Mechanical Behavior of AM Components: Garrett Pataky¹; Benjamin Smith¹; Christopher Laursen²; Jody Bartanus¹; Jay Carroll²; ¹Clemson University; ²Sandia National Laboratories

10:30 AM

Managing Heat Buildup and Standardizing Melt Pool Dimensions in Laser Powder Bed Fusion through a "Powder Moat" Scan Strategy: Evan Diewald¹; Christian Gobert¹; *Jack Beuth*¹; ¹Carnegie Mellon University

10:50 AM

Using Post Build Porosity Analysis to Inform Future Build Strategies: Connor *Varney*¹; Robert Quammen¹; Nicholas Telesz¹; John Balk¹; Andrew Wessman²; Paul Rottmann¹; ¹University of Kentucky; ²University of Arizona

ADDITIVE TECHNOLOGIES

Additive Manufacturing for Energy Applications III — Characterization of **Additive Manufactured Products**



Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Nuclear Materials Committee

Program Organizers: Isabella Van Rooyen, Idaho National Laboratory; Indrajit Charit, University of Idaho; Subhashish Meher, Idaho National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Kumar Sridharan, University of Wisconsin-Madison; Xiaoyuan Lou, Auburn University

Monday AM March 15, 2021

Session Chair: Subhashish Meher, Idaho National Laboratory

8:30 AM Invited Microstructural, Mechanical, and Corrosion Behavior of a High Entropy Alloy (HEA) Designed for Harsh Aqueous Environments: *Nikole Kucza*¹; Martin Morra¹; Kosuke Kuwabara²; ¹GE Global Research; ²Global Research & Innovative Technology Center GRIT

8:50 AM

Microstructural Stability and Creep Behavior of an Additively Manufactured Al-Ce-Ni-Mn Alloy: *Richard Michi*¹; Kevin Sisco²; Sumit Bahl¹; Jonathan Poplawsky¹; Lawrence Allard¹; Ryan Dehoff¹; Alex Plotkowski¹; Amit Shyam²; ¹Oak Ridge National Laboratory; ²University of Tennessee, Knoxville

9:10 AM

Microstructure-property of a Novel 9Cr Ferritic Martensitic Steel via Additive Manufacturing Directed Energy Deposition: *Weicheng Zhong*¹; Lizhen Tan¹; Kevin Field²; Niyanth Sridharan³; Ying Yang¹; Kurt Terrani¹; ¹Oak Ridge National Laboratory;



²University of Michigan, Ann Arbor; ³Lincoln Electric Company

9:30 AM

The Effect of Grain Orientation on Nanoindentation Behavior of Selective Laser Melted Austenitic Stainless Steel: *Sravya Tekumalla*¹; Sudharshan Raman¹; Matteo Seita¹; ¹Nanyang Technological University

9:50 AM

Quality Evaluation of As-printed Wire Arc Additively Manufactured 316L Stainless Steel Blocks: *Yukinori Yamamoto*¹; Lizhen Tan¹; Ying Yang¹; Andrzej Nycz¹; Mark Noakes¹; Yousub Lee¹; Luke Meyer¹; William Carter¹; Thak Sang Byun¹; Ryan Dehoff¹; Kurt Terrani¹; ¹Oak Ridge National Laboratory

10:10 AM

Elevated Temperature Dip in Tensile Elongation of an Additively Manufactured Al-Cu-Ce Alloy: *Sumit Bahl*¹; Kevin Sisco²; Jonathan Poplawsky¹; Richard Michi¹; Lawrence Allard¹; Ryan Dehoff¹; Alex Plotkowski¹; Amit Shyam¹; ¹Oak Ridge National Laboratory; ²University of Tennessee-Knoxville

10:30 AM

Microstructure and Properties Comparison for 316L Wire-fed Laser Metal Deposition AM Under Vacuum Conditions: *Nicholas Brubaker*¹; Nicolene van Rooyen²; Hussam Ali¹; Mark Jaster³; Indrajit Charit¹; Michael Maughan¹; ¹University of Idaho; ² University of Idaho; ³Premier Technology

10:50 AM

Advances in Digital Light Printing for Energy Applications: *Donna Guillen*¹; Patrick Moo¹; Michael Shaltry¹; Robert O'Brien¹; ¹Idaho National Laboratory

Additive Manufacturing of Metals: Applications of Solidification Fundamentals

- Continuum Scale Modeling and Experiments

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Solidification Committee

Program Organizers: Alex Plotkowski, Oak Ridge National Laboratory; Lang Yuan, University of South Carolina; Kevin Chaput, Northrop Grumman; Mohsen Asle Zaeem, Colorado School of Mines; Wenda Tan, University of Utah; Lianyi Chen, University of Wisconsin-Madison

Monday AM March 15, 2021

Session Chairs: Alex Plotkowski, ORNL; Matt Rolchigo, LLNL

8:30 AM

Statistical Modeling of Microstructure Signatures in Laser Powder Bed Fusion: Supriyo Ghosh¹; Raiyan Seede¹; Jaylen James¹; Ibrahim Karaman¹; Alaa Elwany¹; Douglas Allaire¹; Raymundo Arroyave¹; ¹Texas A&M University

8:50 AM

Solidification Behavior of Martensitic Precipitation-hardenable Stainless Steels **Produced via Additive Manufacturing**: *Eric Lass*¹; ¹University of Tennessee, Knoxville

9:10 AM

3D Characterisation of Cracks Formed in AA2024 and Implications for Alloy **Design**: *Giuseppe Del Guercio*¹; Marco Simonelli¹; Nesma Aboulkhair¹; Graham McCartney¹; Chris Tuck¹; ¹University of Nottingham



9:30 AM

Quantification and Propagation of Aleatoric Uncertainty Through Numerical Simulation of Laser Powder Bed Fusion Process for IN625: Scott Wells¹; ¹Purdue University

9:50 AM

Quantifying Impact of Fluid Flow on Melt Pool Model Predictions Across AM **Processing Regimes**: Gerald Knapp¹; Matthew Rolchigo²; Tarasankar DebRoy¹; Jim Belak²; Alex Plotkowski³; ¹The Pennsylvania State University; ²Lawrence Livermore National Laboratory; ³Oak Ridge National Laboratory

10:10 AM

Alternative Scan Strategies for Laser Powder Bed Additive Manufacturing to **Expand Process Space**: *Elizabeth Chang-Davidson*¹; Nicholas Jones¹; Jack Beuth¹; ¹Carnegie Mellon University

10:30 AM

Microstructure Control with Advanced Scan Strategies Developed via Fast Analytic Thermal Modeling of Additive Processes: Benjamin Stump¹; Patxi Fernandez¹; Matt Rolchigo²; Alex Plotkowski¹; Jim Belak²; ¹ORNL; ²LLNL

10:50 AM

Consistent Coupling between Melt Pool Heat Transfer and Grain-scale CA **Calculations for Additive Manufacturing**: John Coleman¹; Alex Plotkowski¹; Matt Rolchigo²; ¹Oak Ridge National Laboratory; ²Lawrence Livermore National Laboratory

ADDITIVE TECHNOLOGIES



Additive Manufacturing: Materials Design and Alloy Development III -- Super

Materials and Extreme Environments — Fundamentals

- - - TMS
- VEBSITE

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek **Innovations LLC**

March 15, 2021 Monday AM

Session Chairs: Behrang Poorganji, Beehive3D; James Saal, Citrine Informatics

8:30 AM

Introductory Comments: Additive Manufacturing: Materials Design and Alloy **Development III -- Super Materials and Extreme Environments**: *Behrang Poorganji*¹; ¹University of Waterloo

8:35 AM Invited AM Enabled Super Materials for Extreme Environments Applications: Youping Gao¹; John Porter¹; Cameron Schmidt¹; ¹Castheon Inc

9:05 AM Invited

Development of a Rapid Alloy Selection Tool for Rapid Solidification Processing **Conditions**: *Emma White*¹; Ralph Napolitano¹; Timothy Prost¹; Duane Johnson¹; Samantha Tatar²; Naren Raghavan³; Michael Kirka³; Andrew Kustas⁴; Nicolas Argibay⁴; IverAnderson¹; ¹Ames Laboratory; ²Kansas City National Security Campus; ³Oak Ridge National Laboratory; ⁴Sandia National Laboratories

9:35 AM

Additive Manufacturing and Characterization of High-density Materials for Aerospace Applications: *Kristyn Kadala*¹; Scott Smith¹; ¹Lockheed Martin ATC

9:55 AM Invited

Computational Design and Additive Manufacturing-Enabled Fabrication of Functionally Graded Steel-to-Tungsten Joints for Fusion Energy Applications: Dana Frankel¹; Marie Thomas¹; Pin Lu¹; Olga Eliseeva²; Tanner Kirk²; Raymundo Arroyave²; Ibrahim Karaman²; ¹QuesTek Innovations LLC; ²Texas A&M University

10:25 AM Invited

Rapid Exploration of Refractory Complex Concentrated Alloys via Additive **Manufacturing and Molecular Dynamics**: Andrew Kustas¹; Jonathan Pegues¹; Michael Melia¹; Raymond Puckett¹; Shaun Whetten¹; Morgan Jones¹; Nicolas Argibay¹; Michael Chandross¹; ¹Sandia National Laboratories

10:55 AM

Application of Taguchi, Response Surface, and Artificial Neural Networks for **Rapid Optimization of Laser-based Powder-Bed Fusion Process**: *Ebrahim Asadi*¹; Behzad Fotovvati¹; Faridreza Attarzadeh¹; ¹University of Memphis

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation – Session I**



Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials Characterization Committee

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Monday AM March 15, 2021

8:30 AM Invited Mechanism of Hardening and Damage Initiation in Oxygen Embrittlement of Body-Centred-Cubic Niobium: *Weizhong Han*¹; ¹Xi'an Jiaotong University

9:00 AM

Evaluation Method of Ductile-to-Brittle Transition Temperature Using Nanoindentation and Molecular Dynamics Simulation: *Yeonju Oh*¹; Won-Seok Ko²; Nojun Kwak¹; Takahito Ohmura³; Heung Nam Han¹; ¹Seoul National University; ²University of Ulsan; ³National Institute for Materials Science

9:20 AM

Migration kinetics of twinning disconnections in nanotwinned Cu: an in situ HRTEM deformation study: *Quan Li*¹; Jian Song¹; GuiSen Liu¹; Yue Liu¹; XiaoQin Zeng¹; ¹Shanghai Jiao Tong University **MOBILE-FRIEND**

9:40 AM

High Angular Resolution EBSD From Spherical Harmonic Transform Indexing: *Gregory Sparks*¹; Mark Obstalecki²; Paul Shade²; Michael Uchic²; Stephen Niezgoda¹; Michael Mills¹; ¹Ohio State University; ²Air Force Research Laboratory

10:00 AM

Kinking in MAX Phases Studied via a Combined Experimental/Computational Approach: *Gabriel Plummer*¹; Garritt Tucker¹; ¹Colorado School of Mines

10:20 AM Studying Dislcoation Interactions in the Bulk Using Dark Field X-ray Microscopy: Henning Friis Poulsen¹; ¹DTU

10:40 AM

Interactions between Dislocations and a Low-angle Grain Boundary in a Single Crystalline CrCoNi Medium-entropy Alloy: Frederic Habiyaremye¹; Antoine Antoine Guitton¹; Florian Schafer²; Felicitas Scholz³; Mike Schneider³; Jan Frenzel³; Guillaume Laplanche³; Nabila Maloufi¹; ¹Université de Lorraine–CNRS–Arts et Métiers ParisTech–LEM3; ²Saarland University; ³Institut für Werkstoffe, Ruhr– Universität Bochum, Universitätsstr. 150

11:00 AM

Electron Microscopy-based Assessment of the Role of Short Range Order on Deformation Behavior of High and Medium Entropy Alloys: Daniel Foley¹; James Hart¹; ElafAnber²; Robert Ritchie³; Andrew Minor³; MarkAsta³; Flynn Walsh⁴; Douglas Spearot⁵; Mitra Taheri¹; ¹Johns Hopkins University; ²Drexel University; ³University of California, Berkeley; ⁴Lawrence Berkeley National Laboratory; ⁵University of Florida



MONDAY AM

Sponsored by: TMS Structural Materials Division, TMS: Steels Committee

Program Organizers: Ana Luiza Araujo, CBMM North America Inc.; Louis Hector, General Motors Global Technical Center; Igor Vieira, Nucor Steel; Lijia Zhao, ArcelorMittal USA; Krista Limmer, CCDC Army Research Laboratory; Jonah Klemm-Toole, Colorado School of Mines; Sebastien Allain, Institut Jean Lamour; MingXin Huang, University of Hong Kong

Monday AM March 15, 2021

8:30 AM

Ferrite Recrystallization Investigated by In Situ High Energy X-ray Diffraction Experiments: *Clélia Couchet*¹; Sébastien Allain¹; Julien Teixeira¹; Marc Moreno²; Guillaume Geandier¹; Frédéric Bonnet³; ¹Institut Jean Lamour; ²Transvalor S.A.; ³ArcelorMittal

8:50 AM

Carbon Content in Carbide-free Bainite during Isothermal Transformations: Irina Pushkareva¹; Babak Shalchi-Amirkhiz¹; *Sebastien Allain*²; Guillaume Geandier²; Frédéric Danoix³; Fateh Fazeli¹; Matthew Sztanko¹; Colin Scott¹; ¹CanMet Materials - Natural Resources Canada; ²Institut Jean Lamour; ³Groupe de Physique des Matériaux

9:10 AM

Dislocation Densities during Martensite Transformation in a Low-carbon Steel Determined by In Situ High Energy X-ray Diffraction: *Juan Macchi*¹; Steve Gaudez¹; Guillaume Geandier¹; Julien Teixeira¹; Sabine Denis¹; Frédéric Bonnet²; Sébastien Allain¹; ¹Institut Jean Lamour; ²ArcelorMittal Research SA



9:30 AM

Effect of Phase Stability of Retained Austenite during Deformation in Lowalloy Multiphase Steels: *Avala Lavakumar*¹; Myeong-heom PARK¹; Hiroki Adachi²; Masugu Sato³; Nobuhiro Tsuji¹; ¹Kyoto University; ²University of Hyogo; ³Japan Synchrotron Radiation Research Institute (JARSI), Sayo-gun, Hyogo

9:50 AM

Microstructural and Plastic Deformation Study of a Multi-phase Advanced High Strength Steel: AFM Monowar Hossain¹; *Nilesh Kumar*; ¹University of Alabama Tuscaloosa

10:10 AM

Strain Rate Sensitive Martensite Transformation in a Q&P Steel: *Christopher Finfrock*¹; Melissa Thrun¹; Trevor Ballard¹; John Copley¹; Benjamin Ellyson¹; Amy Clarke¹; Kester Clarke¹; ¹Colorado School of Mines

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Energy Conversion and Storage I

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

VEBSIT

TMS



NTENTS



Session Chairs: Jung Pyung Choi, Pacific Northwest National Laboratory; Partha Mukherjee, Purdue University

8:30 AM Keynote Infiltration Strategies to Improve the Performance of Solid Oxide Fuel Cell **Anodes**: Soumendra Basu¹; Boshan Mo¹; Jillian Rix¹; Srikanth Gopalan¹; Uday Pal¹; ¹Boston University

9:10 AM Keynote Thermal Implications of Diverging Degradation Modes in Battery Electrodes and **Opportunities to Enable Anode-free Systems**: *Corey Love*¹; Rachel Carter¹; Robert Atkinson²; Todd Kingston³; ¹US Naval Research Laboratory; ²EXCET, Inc.; ³NRC/ NRL Postdoctoral Research Associate

9:50 AM Keynote Designing Electrode Architectures across Length Scales: Some Lessons Learned from Li-ion and "Beyond Li" Chemistries: Sarbajit Banerjee¹; ¹Texas A&M University

CHARACTERIZATION

Advanced Real Time Imaging — Additive Manufacturing

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

March 15, 2021 Monday AM

Session Chairs: David Veysset, Stanford University; Jinichiro Nakano, USDOE National Energy Technology Laboratory

8:30 AM

An In Situ and Operando Additive Manufacturing Process Replicator for High Speed Optical, Infra-red and Synchrotron X-ray Imaging: Sebastian Marussi¹; Chu Lun Alex Leung¹; Samuel Clark¹; Leigh Stranger²; Robert Atwood³; Veijo Honkimäki⁴; Alexander Rack⁴; Mike Besston⁵; Jon Willmott²; Peter Lee¹; ¹University College London; ²The University of Sheffield; ³Diamond Light Source Ltd; ⁴European Synchrotron Radiation Facility; ⁵Oxford Lasers Ltd

8:50 AM

In Situ Characterization of the Balling Phenomenon in Additive Manufacturing: *Debomita Basu*¹; Jack Beuth¹; Bryan Webler¹; ¹Carnegie Mellon University

9:10 AM

In-Situ Machine Learning Enabled Spatter Detection in Laser Powder Bed Fusion Additive Manufacturing: Brandon Abranovic¹; Jack Beuth¹; Rishikesh Magar¹; Lalit

Ghule¹; Amir Farimani¹; ¹Carnegie Mellon University

- TMS WEBSITE

9:30 AM

High-speed Synchrotron X-ray Imaging of Metal Additive Manufacturing Processes: *Tao Sun*¹; Kamel Fezzaa²; ¹University of Virginia; ²Argonne National Laboratory

9:50 AM Invited

Characterizing Laser-Driven Metal Ejecta Interactions: *Alison Saunders*¹; Camelia Stan¹; Kyle Mackay¹; Suzanne Ali¹; Hans Rinderknecht²; Hye-Sook Park¹; Jon Eggert¹; Fady Najjar¹; Tomorr Haxhimali¹; Brandon Morgan¹; Marcho Echeverria³; Jeremy Horwitz¹; Yuan Ping¹; ¹Lawrence Livermore National Laboratory; ²Laboratory for Laser Energetics; ³University of Connecticut

10:10 AM

Quantifying Spatter in Powder Bed Fusion Processes with High-Speed Video Observations and Machine Learning: *Christian Gobert*¹; Evan Diewald¹; Jack Beuth¹; ¹Carnegie Mellon University

MATERIALS PROCESSING

Advances in Powder and Ceramic Materials Science — Structure Design and Processing

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Materials Characterization Committee, TMS: Powder Materials Committee

Program Organizers: Bowen Li, Michigan Technological University; Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology; Kathy Lu, Virginia Polytechnic Institute and State University; Rajiv Soman, Eurofins EAG Materials Science LLC; Faqin Dong, Southwest University of Science and Technology; Jinhong Li, China University of Geosciences (Beijing); Ruigang Wang, The University of Alabama; Eugene Olevsky, San Diego State University



MONDAY AM

NTENTS

Π

O

Monday AM March 15, 2021

Session Chairs: Ruigang Wang, The University of Alabama; Jinhong Li, China University of Geosciences (Beijing)

8:30 AM Invited Structural Integrity of Complex Oxide Scales for Improved Oxidation Resistance of Ultra-high Temperature Ceramics: *Ambreen Nisar*¹; Cheng Zhang¹; Benjamin Boesl¹; Arvind Agarwal¹; ¹Florida International University

8:50 AM Invited

New Insights into Sintering Processing for Solid State Electrolytes – A Phase-Field Simulation Study

: *Rongpei Shi*¹; Marissa Wood¹; Jose Espitia¹; Xiaosi Gao²; Joshua Hammons¹; LiWen Wan¹; Shin Young Kang¹; Dive Mukund¹; Kwangnam Kim¹; Tae Wook Heo¹; Brandon Wood¹; Jianchao Ye¹; ¹Lawrence Livermore National Laboratory; ²Cornell University

9:10 AM

Flash Sintering of Gadolinium-doped Ceria: Densification and Microstructure: *Tarini Prasad Mishra*¹; Viviana Avila²; Rubens Roberto Ingraci Neto²; Rishi Raj²; Olivier Guillon¹; Martin Bram¹; ¹Forschungszentrum Jülich GmbH; ²University of Colorado Boulder

9:30 AM

Processing of TiB2-TiC Based Materials with Fine Microstructure and Improved

Mechanical Properties: *Zhezhen Fu*¹; ¹University of Wisconsin Platteville

9:50 AM

Discovery of Novel High-entropy Ceramics via Machine Learning: *Kevin Kaufmann*¹; William Mellor¹; Tyler Harrington¹; Chaoyi Zhu¹; Alexander Rosengarten¹; Daniel Maryanovsky¹; Kenneth Vecchio¹; ¹University of California, San Diego

10:10 AM

Elucidating the Influence of the Thermodynamics, Kinetics, and Chemistries of Molten Salts to Synthesize Ceramics for Energy Applications: *Benjamin Levitas*¹; Katsuyoshi Kakinuma²; Srikanth Gopalan¹; ¹Boston University; ²University of Yamanashi

10:30 AM

Effects of Yttria Content and Atmosphere on Structural Evolution of Highly Porous Yttria-stabilized Zirconia Aerogels: *Nathaniel Olson*¹; Frances Hurwitz²; Haiquan Guo³; Jessica Krogstad¹; ¹University of Illinois Urbana Champaign; ²NASA Glenn Research Center; ³Ohio Aerospace Institute

MATERIALS DESIGN

AI/Data Informatics: Applications and Uncertainty Quantification at Atomistics and Mesoscales — Session I

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid



MONDAY AM

TABLE

Q

NTENTS

Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Monday AM March 15, 2021

Session Chairs: Ghanshyam Pilania, LANL; Garvit Agarwal, ANL

8:30 AM

Are We Making Progress on ML Algorithms for Structure-property Relationships? Using MatBench as a Test Bed: *Anubhav Jain*¹; ¹Lawrence Berkeley National Laboratory

9:00 AM

Model Comparison and Uncertainty Prediction for ML Models of Crystalline Solids Material Properties: *Francesca Tavazza*¹; Kamal Choudhary¹; Brian De Cost¹; ¹NIST

9:30 AM

Data Science Approaches to Develop Predictive Models for Energy-relevant Materials: *Badri Narayanan*¹; ¹University of Louisville

10:00 AM

Discovery and Classification of Double Spinel Chemical Space: *Ghanshyam Pilania*¹; Vancho Kocevski¹; Blas Uberuaga¹; ¹Los Alamos National Laboratory

10:30 AM

Inverse Design of Energy Storage Materials via Active Learning: *Hieu Doan*¹; Garvit Agarwal¹; Rajeev Assary¹; ¹Argonne National Laboratory

10:50 AM

Accelerating the Discovery of Self-Reporting Redox-active Materials Using

TMS



MATERIALS DESIGN



CONTENTS TABLE **O**

MOBILE-FRIENDL

Algorithm Development in Materials Science and Engineering — Machine Learning and Atomistic Algorithms to Accelerate Materials Study and Design

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Monday AM March 15, 2021

Session Chairs: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, Ames Laboratory

8:30 AM Invited Theory-infused Machine Learning Algorithms of Chemisorption at Metal Surfaces: Hongliang Xin¹; ¹Virginia Polytechnic Institute and State University

9:00 AM Invited Accelerating Atomistic Monte Carlo Simulations with Autoregressive Models: *Rafael Gomez-Bombarelli*¹; James Damewood¹; ¹Massachusetts Institute of Technology

9:30 AM

Application of a Shape Moment Descriptor Set Towards a Robust and Transferable **Description of Local Atomic Environments**: *Jacob Tavenner*¹; Edward Kober²; Garritt Tucker¹; ¹Colorado School of Mines; ²Los Alamos National Laboratory

9:50 AM Invited High Speed Artificial Neural Network Implementation of Interatomic Force Fields in Metals: Doyl Dickel¹; Christopher Barrett¹; Mashroor Nitol¹; ¹Mississippi State University

10:20 AM

Machine Learning and Supercomputing to Accelerate the Development of **ReaxFF Interatomic Potentials**: *N. S. Harsha Gunda*¹; Jian Peng¹; Yun Kyung Shin²; Sangkeun Lee¹; Adri C. T. Van Duin²; Dongwon Shin¹; ¹Oak Ridge National Laboratory; ²Pennsylvania State University

10:40 AM

Development of Machine Learned SNAP Potentials for Studying Radiation **Damage in Materials**: *Mary Alice Cusentino*¹; Mitchell Wood¹; Aidan Thompson¹; ¹Sandia National Laboratories

11:00 AM

Computational Synthesis of Substrates by Crystal Cleavage: Joshua Paul¹; Alice Galdi²; Richard Hennig¹; ¹University of Florida; ²Cornell University

ELECTRONIC MATERIALS

Alloys and Compounds for Thermoelectric and Solar Cell Applications IX —



VEBSITE TMS



MONDAY AM

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Alloy Phases Committee**

Program Organizers: Hsin-Jay Wu, National Chiao Tung University; Sinn-wen Chen, National Tsing Hua University; Franck Gascoin, Cnrs Crismat Unicaen; Philippe Jund, Montpellier University; Yoshisato Kimura, Tokyo Institute of Technology; Lan Li, Boise State University; Takao Mori, National Institute for Materials Science; Tiejun Zhu, Zhejiang University; Alexandra Zevalkink, Michigan State University; Wan-Ting Chiu, Tokyo Institute of Technology

March 15, 2021 Monday AM

Session Chairs: Hsin-Jay Wu, National Chiao-Tung University; Albert T. Wu, National Central University

8:30 AM Introductory Comments: Alloys and Compounds for Thermoelectric and Solar **Cell Applications IX**: *Hsin-Jay Wu*¹; ¹National Chiao Tung University

8:35 AM Invited n-Bi2-xSbxTe3 as an Alternative to Mainstream n-Bi2Te3-xSex Near Room **Temperature**: *Jian He*¹; Lipeng Hu²; ¹Clemson University; ²Shenzhen University

8:55 AM Invited Enhanced Thermoelectric Figure-of-Merit in Nanostructured n-type Bi2Te3 via **Phase Diagram Engineering**: Hsin-Ching Huang¹; Wan-Ting Yen²; *Hsin-Jay Wu*²; ¹National Sun Yat-sen University; ²National Chiao Tung University

9:15 AM Invited

Unique Influences of Laser Additive Manufacturing on Multiscale Structuring of Bismuth Telluride Thermoelectric Materials: Saniya Leblanc¹; Ryan Welch¹; Bengisu Sisik¹; ¹George Washington University

9:35 AM Invited Assessment of Electroless Cobalt Diffusion Layer for Bi, Te, -based Thermoelectric Module: Albert T. Wu¹; Chun-Hsien Wang¹; ¹National Central University

9:55 AM

Effect of Interfacial Reaction on Bi2Te3 and Sb2Te3 Thin-film Thermoelectric Module: Kai-Wen Cheng¹; Zhen-Wei Sun¹; Albert T. Wu¹; ¹National Central University

10:15 AM

Thermomagnetic Properties of Single-crystal 2H-NbSe, and Bi, Te, Md Sabbir Akhanda¹; S. Emad Rezaei¹; Md Golam Rosul¹; Keivan Esfarjani¹; Sergiy Krylyuk²; Albert Davydov²; Mona Zebarjadi¹; ¹University of Virginia; ²National Institute of Standards and Technology

BIOMATERIALS

Bio-Nano Interfaces and Engineering Applications — Bio-Nano I



Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Biomaterials Committee**

Program Organizers: Candan Tamerler, University of Kansas; Kalpana Katti, North Dakota State University; Hendrik Heinz, University of Colorado Boulder; Terry Lowe, Colorado School of Mines; Po-Yu Chen, National Tsing Hua University

Monday AM March 15, 2021

Session Chairs: Candan Tamerler, Uniersity of Kansas; KAlpana Katti, North Dakota State University

8:30 AM Invited **Bio-imaging with Photoluminescence of Single-layer MoS2**: Yuhei Hayamizu¹; ¹Tokyo Institute of Technology

9:00 AM Invited Stickiness at Bio-nano-interfaces: From Nanoscale Characterization to Macroscale Properties: Hannes Schniepp¹; ¹College of William & Mary

9:30 AM Invited Insight into the Mechanobiological Progression of Cancer Metastasis to Bone: *Dinesh Katti*¹; Sharad Jaswandkar¹; Kalpana Katti¹; ¹North Dakota State University

10:00 AM

Control of Scaffold Shear Forces Through a Perfusion Bioreactor for Design of **Prostate Cancer Bone Metastasis Testbed**: *Haneesh Jasuja*¹; Akerkouch Lahcen¹;



CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Advanced **Characterization Methods I**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

Monday AM March 15, 2021

Session Chairs: Alex Moser, U.S. Naval Research Laboratory; Juan Escobedo-Diaz, University of New South Wales

8:30 AM

Performance of High Fidelity Inert Thermomechanical Mocks Over a Diverse Range of Strain Rates and Temperatures: *Alexandra Burch*¹; Benjamin Morrow¹; Carl Cady¹; David Bahr²; John Yeager¹; ¹Los Alamos National Laboratory; ²Purdue University



8:50 AM

Microstructure Characterization of Aluminum 1100 Using Ultrasonic Backscatter Measurements and Synthetic Polycrystals: *Musa Norouzian*¹; Joseph Turner¹; ¹University of Nebraska-Lincoln

9:10 AM

A Lightweight Mossbauer Spectrometer for Lunar Exploration Using a Piezoelectric Doppler Drive: *Pedro Guzman*¹; Stefan Lohaus¹; Valerie Scott²; Brent Fultz¹; ¹California Institute of Technology; ²Jet Propulsion Laboratory, California Institute of Technology

9:30 AM

SAXS Tomography of Precipitation Hardened Multilayer Al Alloy Sheets: Shan Lin¹; Hiroshi Okuda¹; ¹Kyoto University

9:50 AM

APT Composition Profiling for Accurate Evaluation of Diffusion Coefficients in the Zr-Ta Binary System: Yaqiao Wu¹; Megha Dubey¹; Shujuan Wang¹; Chuangye Wang²; Ji-Cheng Zhao²; ¹Boise State University; ²University of Maryland

10:10 AM

Large-scale Crystal Orientation Mapping by Directional Reflectance Microscopy: Matteo Seita¹; Xiaogang Wang¹; Mallory Wittwer¹; ¹Nanyang Technological University

10:30 AM

Utilization of Magneto-optical Kerr Effect Microscopy for Microstructural Characterization of Steels: *Matic Jovicevic-Klug*¹; Patricia Jovicevic-Klug¹; Lars Thormählen²; Jeffrey McCord²; Bojan Podgornik¹; ¹Institute of Metals and



MONDAY AM

CONTENTS

TABLE OF

Technology; ²Institute for Materials Science, Kiel University

10:50 AM Characterization of Dealloyed Gradient Nanoporous Foams: Karina Hemmendinger¹; Andrea Hodge¹; ¹University of Southern California

NUCLEAR MATERIALS

Characterization of Nuclear Materials and Fuels with Advanced X-ray and Neutron Techniques — X-ray Diffraction/Scattering I

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Nuclear Materials Committee

Program Organizers: Xuan Zhang, Argonne National Laboratory; Jonathan Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University; Joshua Kane, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory; J. Kennedy, Idaho National Laboratory; Arthur Motta, Pennsylvania State University

Monday AM March 15, 2021

Session Chairs: Jonathan Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University

8:30 AM Invited Synchrotron High-energy X-ray Studies of Nuclear Reactor Materials: *Meimei Li*¹; Xuan Zhang¹; Jonathan Almer¹; Jun-Sang Park¹; Peter Kenesei¹; Andrew Chuang¹;

TMS



MOBILE-FRIENDL

CONTENTS

TABLE

Q

Evolution of Stresses in Deformation Twins in the Plastic Zone Using Threedimensional Synchrotron X-ray Diffraction: Hamidreza Abdolvand¹; Karim Louca¹; Charles Mareau²; Marta Majkut³; Jonathan Wright³; ¹Western University; ²Arts et Métiers ParisTech; ³European Synchrotron Radiation Facility (ESRF)

9:20 AM

9:00 AM

Characterization of Long Range Ordering in Ni-based Alloys with Ex-situ and Insitu Synchrotron X-ray Diffraction: Nicholas Aerne¹; David Sprouster²; Fei Teng³; Mehmet Topsakal⁴; Adrien Couet⁵; Kumar Sridharan⁵; Julie Tucker¹; ¹Oregon State University; ²Stony Brook University; ³Idaho National Lab; ⁴Brookhaven National Lab; ⁵University of Wisconsin-Madison

9:40 AM

Irradiation-induced Effects in HT-UPS Steel Using Far-field X-ray Diffraction and Grain Tracking Analysis: Sri Tapaswi Nori¹; Alejandro Figueroa¹; Jonova Thomas¹; Hemant Sharma²; Jun-Sang Park²; Peter Kenesei²; Jonathan Almer²; Maria Okuniewski¹; ¹Purdue University; ²Argonne National Laboratory

10:00 AM Invited

MultimodalSynchrotronCharacterizationofTransmutationProductsinStructural **Materials**: *David Sprouster*¹; J Trelewicz¹; D Morrall²; X Hu²; C Parish²; B Wirth³; Y Katoh²; L Snead¹; ¹Stony Brook University; ²ORNL; ³University of Tennessee, Knoxville

10:30 AM

4D X-ray Diffraction Microscopy Study of Tensile Deformation of Neutronirradiated Fe-9Cr Alloy: Xuan Zhang¹; Dominic Piedmont²; Jun-Sang Park¹; Peter Kenesei¹; Jonathan Almer¹; Meimei Li¹; ¹Argonne National Laboratory; ²University



MONDAY AM

of Illinois at Urbana-Champaign

10:50 AM In-Situ XRD Study of Alloy 709's Mechanical Behavior for Advanced Fast Reactor Applications: *Dominic Piedmont*¹; Donghee Park¹; Victoria Riso¹; Xiang Liu¹; James Stubbins¹; ¹University of Illinois at Urbana Champaign

CORROSION

Coatings and Surface Engineering for Environmental Protection III — **Protection from Environmental Degradation, Session I**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Arif Mubarok, PPG; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University; Mary Lyn Lim, PPG Industries; Raul Rebak, GE Global Research; Brian Okerberg, PPG Industries

Monday AM March 15, 2021

8:30 AM

Revealing the Long-term Growth Kinetics and Morphology of Atmospheric **Corrosion Pitting in Aluminum via In-operando Microtomography**: *Philip Noell*¹; Michael Melia¹; Eric Schindelholz²; ¹Sandia National Laboratories; ²The Ohio State University

8:50 AM



Program Organizers: Anne Campbell, Oak Ridge National Laboratory; Dong

Thomas Watson²; Tod Policandriotes³; Mark Aindow¹; ¹University of Connecticut; ²Pratt & Whitney; ³Collins Aerospace

9:10 AM

The Effect of Surface Treatment on the Formation, Structure, and Chemistry of Protective Oxide Scale on High-temperature Oxidation-resistant Nickel Alloys: Stephen House¹; Henry Ayoola¹; John Lyons¹; Meng Li¹; Bingtao Li¹; Judith Yang¹; Wissam Saidi¹; Brian Gleeson¹; ¹University of Pittsburgh

9:30 AM

Cycling Corrosion Testing of Al-Mg Friction Stir Welding Bi-metallic Joints: Qingli *Ding*¹; Brajendra Mishra¹; Adam C Powell¹; Kübra Karayagiz¹; ¹Worcester Polytechnic Institute

9:50 AM

Dealloying and Passivation of Cu-doped Carbide-reinforced Martensitic Steels in a Sulfuric Acid: Kenta Yamanaka¹; Manami Mori²; Kazuo Yoshida¹; Kazuyo Omura¹; Yusuke Onuki³; Shigeo Sato³; Akihiko Chiba¹; ¹Tohoku University; ²National Institute of Technology, Sendai College; ³Ibaraki University

NUCLEAR MATERIALS

Composite Materials for Nuclear Applications – TRISO Fuel

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee, TMS: Nuclear Materials Committee



Liu, University of Bristol; Rick Ubic, Boise State University; Lauren Garrison, Oak Ridge National Laboratory; Peng Xu, Idaho National Laboratory; Johann (Hans) Riesch, Max Planck Institute for Plasma Physics

March 15, 2021 Monday AM

Session Chair: Dong Liu, University of Bristol

8:30 AM Invited Tristructural Isotropic (TRISO) Fuel for High-Temperature, Passively-Safe Nuclear Reactors: John Stempien¹; Paul Demkowicz¹; John Hunn²; ¹Idaho National Laboratory; ²Oak Ridge National Laboratory

9:00 AM

Experimental Characterisation of the Variation of Local Residual Stresses in **TRISO Coatings**: *Alex Leide*¹; Steven Knol²; Arjan Vreeling²; Dave Goddard³; Dong Liu¹; ¹University of Bristol; ²NRG; ³National Nuclear Laboratory

9:20 AM

Post-irradiation Examinations of TRISO Particles Corroded in Molten FLiBe **Salt under Neutron Irradiation**: *Guiqiu Zheng*¹; David Carpenter¹; ¹Massachusetts Institute of Technology

MATERIALS DESIGN

Computational and Modeling Challenges in Metals and Alloys for Extreme Environments — Extreme Environment Simulations from Nano- to Macro-scale



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Jean-Briac le Graverend, Texas A&M University; Jaafar El-Awady, Johns Hopkins University; Giacomo Po, University of Miami; Beñat Gurrutxaga-Lerma, University of Birmingham

Monday AM March 15, 2021

Session Chairs: Jean-Briac le Graverend, Texas A&M University; Avinash Dongare, University of Connecticut

8:30 AM

Molecular Dynamics Modeling of the Influence of Magnesium Dopants on Grain Boundary Stabilization in Nanocrystalline Aluminum: Wenye Ye¹; Leslie Mushongera¹; ¹University of Nevada, Reno

8:50 AM

Understanding Interface Properties Through Dislocation Dynamics Simulations in Metallic Nanolaminates: Aritra Chakraborty¹; Miroslav Zecevic¹; Abigail Hunter¹; Xiang-Yang Liu¹; Ricardo Lebensohn¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

9:10 AM

A Thermo-mechanical Model of the Dynamics of Dislocation Fields in Transient Heterogeneous Temperature Fields: Manas Upadhyay¹; ¹LMS, CNRS, Ecole MONDAY AM



Polytechnique, Institut Polytechnique de Paris

9:30 AM

Multi-scale Simulations of Crystallographic Facet-orientation Dependent **Corrosion Behavior in Metallic Alloys**: *Rongpei Shi*¹; Stephen Weitzner¹; Tim Hsu¹; Xiao Chen¹; Tae Wook Heo¹; Tuan Pham¹; Christine Orme¹; Morris Wang¹; Brandon Wood¹; ¹Lawrence Livermore National Laboratory

9:50 AM

The Role of Precipitates on the Microstructure-sensitive Creep Response of 347H Steel via Crystal Plasticity Simulations: Veerappan Prithivirajan¹; Nathan Beets¹; Aritra Chakraborty¹; M Arul Kumar¹; Ricardo Lebensohn¹; Laurent Capolungo¹; ¹Los **Alamos National Laboratory**

10:10 AM

Lattice Orientation Effect on Intragranular Void Growth in Single- and Polycrystalline Metals: Paul Christodoulou¹; Sylvain Dancette²; Ricardo Lebensohn³; Eric Maire²; Irene Beyerlein¹; ¹University of California, Santa Barbara; ²Institut National des Sciences Appliquées de Lyon; ³Los Alamos National Laboratory

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics – Grain Boundary Properties and Kinetics



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

March 15, 2021 Monday AM

Session Chairs: Reza Darvishi Kamachali, Federal Institute for Materials Research and Testing (BAM); Brandon Runnels, University of Colorado; Ian Winter, Lawrence Livermore National Laboratory; Nana Ofori-Opoku, Canadian **Nuclear Laboratories**

8:30 AM Introductory Comments: Computational Thermodynamics and Kinetics: Nana *Ofori-Opoku*¹; ¹Canadian Nuclear Laboratories

8:35 AM

Extracting and Examining the Grain Boundary Diffusivity Tensor of Hydrogen in Nickel Using Atomistic Simulations: David Page¹; Hadley Peay¹; Katie Varela¹; Oliver Johnson¹; David Fullwood¹; Eric Homer¹; ¹Brigham Young University

8:55 AM Invited

Elastic Interactions in Grain Boundary Phase Transformations: Ian Winter¹; Robert Rudd¹; Tomas Oppelstrup¹; Timofey Frolov¹; ¹Lawrence Livermore National



Laboratory

9:25 AM

Atomistic Modeling of Carbon Atom Redistribution in the Fe-C Martensite: Helena Zapolsky¹; Felix Schwab¹; *Gilles Demange*²; Frederic Danoix¹; Renaud Patte¹; Armen Khachaturyan³; ¹Cnrs, Gpm, Umr 6634; ²Cnrs-University of Rouen Normandy; ³Rutgers University

9:45 AM Invited **Density-based Thermodynamics of Microstructure Defects**: Lei Wang¹; *Reza* Darvishi Kamachali¹; ¹Federal Institute for Materials Research and Testing (BAM)

PHYSICAL METALLURGY

Continuous Phase Transformations – Session I

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee

Program Organizers: Jessica Krogstad, University of Illinois at Urbana-Champaign; Gregory Thompson, University of Alabama; Matthew Steiner, University of Cincinnati; Janelle Wharry, Purdue University

Monday AM March 15, 2021

Session Chairs: Jessica Krogstad, University of Illinois at Urbana-Champaign; Gregory Thompson, University of Alabama



CONTENTS

TABLE

ę

8:30 AM Invited **Cluster Variation Model of Phase Behavior in Heusler-forming Alloy Systems:** *Michael Widom*¹; ¹Carnegie Mellon University

9:00 AM Invited Interfacial Spinodals: *Reza Darvishi Kamachali*¹; ¹Federal Institute for Materials Research and Testing (BAM)

9:30 AM

Competitive Partitioning and Decomposition Evolution in Nanocrystalline Alloys: Gregory Thompson¹; Xuyang Zhou²; Reza Kamachali³; Jaber Mianroodi⁴; Alisson Kwiatkowski da Silva⁴; Pratheek Shanthraj⁵; Dirk Ponge⁴; Baptiste Gault⁴; Bob Svendsen⁶; Dierk Raabe⁴; Brad Boyce⁷; Blythe Clark; Blythe Clark; Blythe Clark⁷; ¹University of Alabama; ²Max-Planck-Institut für Eisenforschung; ³Federal Institute for Materials Research and Testing (BAM); ⁴Max-Planck-Institut für Eisenforschung; ⁵The University of Manchester; ⁶Aachen University; ⁷Sandia National Laboratories

9:50 AM

Study of Precipitation Behavior of High-Cr Ni-based Filler Metals Using In-situ **S/TEM**: Cheng-Han Li¹; Sriram Vijayan¹; Carolin Fink¹; Joerg Jinschek¹; ¹The Ohio **State University**

10:10 AM Invited

Microstructural Engineering of Ni-based Superalloys Processed by Conventional and Additive Manufacturing: Felix Theska¹; Nima Haghdadi¹; Sophie Primig¹; ¹University of New South Wales

10:40 AM

Phase Competition in the Two Steps Continuous Phase Transformation during



MONDAY AM

Solidification of Terbium: *Huajing (Wilson) Song*¹; M.I. Mendelev²; ¹Physics and Chemistry of Materials, Los Alamos National Lab; ²Ames Laboratory, US Department of Energy

CORROSION

Corrosion in Heavy Liquid Metals for Energy Systems – Materials Compatibility with Liquid Metal Coolants I

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Nuclear Materials Committee

Program Organizers: Osman Anderoglu, University of New Mexico; Alessandro Marino, SCK-CEN; Michael Short, Massachusetts Institute of Technology; Peter Hosemann, University of California; Mike Ickes, Westinghouse Electric Company

March 15, 2021 Monday AM

Session Chairs: Alessandro Marino, SCK-CEN; Michael Short, MIT

8:30 AM

Material Needs and Developments for the Westinghouse Lead Fast Reactor: *Mike Ickes*¹; Arash Parsi¹; Luke Czerniak¹; Paolo Ferroni¹; ¹Westinghouse Electric Company

8:50 AM Invited

Compatibility of Alumina-forming Austenitic Steels in Static and Flowing Pb: *Bruce Pint*¹; Jiheon Jun¹; Michael Brady¹; Yuki Yamamoto¹; Michael Ickes²; ¹Oak Ridge National Laboratory; ²Westinghouse Electric Company



Corrosion Behaviour and Microstructural Stability of Alumina-forming Austenitic

9:15 AM

Fundamental Interactions of Steels and Nickel-based Alloys with Lead-based Liquid Alloys or Liquid Tin: Carsten Schroer¹; ¹Karlsruhe Institute of Technology (KIT)

9:35 AM Invited

Exposure Tests of Different Materials in Liquid Lead for LFRs: Effect of the **DissolvedOxygenonCorrosion**: Serena Bassini¹; Camillo Sartorio¹; Andrea Antonelli¹; Sebastiano Cataldo¹; Angela Fiore¹; Massimo Angiolini¹; Daniele Martelli¹; Micheal Ickes²; Paolo Ferroni²; Ivan Di Piazza¹; Mariano Tarantino¹; ¹ENEA; ²Westinghouse **Electric Company**

10:00 AM Invited

Corrosion of Refractory Metals and Advanced Steels in Lead-bismuth Eutectic: *Stuart Maloy*¹; Keith Woloshun¹; Eric Olivas¹; Robert Wahlen²; Terry Grimm²; ¹Los Alamos National Laboratory; ²Niowave Inc.

10:25 AM

Corrosion Investigations of Materials in Antimony-tin and Antimony-bismuth Alloys For Liquid Metal Batteries: *Tianru Zhang*¹; Annette Heinzel¹; Adrian Jianu¹; Alfons Weisenburger¹; Georg Müller¹; ¹Karlsruhe Institute of Technology

10:45 AM

Lead Bismuth Eutectic Corrosion on Austenitic Stainless Steel: Peter Hosemann¹; Konstanza Lambrinou¹; David Frazer¹; Erich Stergar¹; ¹University of California Berkeley

11:05 AM

OF

MONDAY AM



Steels Exposed to Oxygen-containing Molten Lead: Annette Heinzel¹; Adrian Jianu¹; Alfons Weisenburger¹; Hao Shi¹; Renate Fetzer¹; Georg Müller¹; ¹Karlsruher Institut of Technology

11:25 AM

Liquid Metal Embrittlement of Al-containing High-entropy Alloys Exposed to Lead-bismuth Eutectic: *Xing Gong*¹; ¹Shenzhen University

CHARACTERIZATION

Data Science and Analytics for Materials Imaging and Quantification — Session I: Data-led Approaches for 2D Characterization & EBSD

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Emine Gulsoy, Northwestern University; Charudatta Phatak, Argonne National Laboratory; Stephan Wagner-Conrad, Carl Zeiss Microscopy; Marcus Hanwell, Brookhaven National Laboratory; David Rowenhorst, Naval Research Laboratory; Tiberiu Stan, Northwestern University

Monday AM March 15, 2021

Session Chair: Emine Gulsoy, Northwestern University

8:30 AM Introductory Comments: Data Science and Analytics for Materials Imaging and

Quantification: *Emine Gulsoy*¹; ¹Northwestern University

8:35 AM

Computer Vision and Machine Learning for Microstructural Characterization and Analysis: *Elizabeth Holm*¹; Ryan Cohn¹; Nan Gao¹; Katelyn Jones¹; Bo Lei¹; Srujana Yarasi¹; ¹Carnegie Mellon University

9:00 AM

Microstructure Image Segmentation with Deep Learning: from Supervised to Unsupervised Methods: *Bo Lei*¹; Elizabeth Holm¹; ¹Carnegie Mellon University

9:20 AM

ImprovedEBSDIndexingthroughNon-LocalPatternAveraging:DavidRowenhorst¹; Patrick Brewick¹; ¹Naval Research Laboratory

9:45 AM

Resolving Pseudosymmetry in Tetragonal ZrO₂ Using EBSD with a Modified Dictionary Indexing Approach: *Edward Pang*¹; Peter Larsen¹; Christopher Schuh¹; ¹Massachusetts Institute of Technology

10:05 AM Dictionary Indexing of EBSD Patterns Assisted by Convolutional Neural Network: *Zihao Ding*¹; Marc Graef¹; ¹Carnegie Mellon University

10:25 AM

Advancements in EBSD Using Machine Learning: *Kevin Kaufmann*¹; Chaoyi Zhu¹; Alexander Rosengarten¹; Daniel Maryanovsky¹; Tyler Harrington¹; Hobson Lane²; ¹University of California, San Diego; ²Tangible AI LLC

CONTENTS

TABLE

9



MOBILE-FRIEND

Deformation Induced Microstructural Modification — Session I: Deformation of Pure Metals and Model Alloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

Monday AM March 15, 2021

Session Chair: Arun Devaraj, Pacific Northwest National Laboratory

8:30 AM

Introductory Comments: Deformation Induced Microstructural Modification: *Arun Devaraj*¹; ¹Pacific Northwest National Laboratory

8:35 AM Invited

Phase Evolution in Two-phase Alloys during Severe Plastic Deformation: Nirab Pant¹; Nisha Verma¹; Yinon Ashkenazy¹; *Pascal Bellon*¹; Robert Averback¹; ¹University of Illinois at Urbana-Champaign

9:05 AM

Extreme Shear-deformation-induced Modification of Defect Structures and Hierarchical Microstructure in Immiscible Alloy: *Bharat Gwalani*¹; Matthew Olszta¹; Anqi Yu²; Krassimir Bozhilov²; Soumya Varma³; Siddhartha Pathak³; Aashish Rohatgi¹; Suveen Mathaudhu¹; Peter Sushko¹; Cynthia Powell¹; Arun Devaraj¹; ¹Davife Nerthwest National Laboratory ² University of California Diversides ³ Power

TMS

¹Pacific Northwest National Laboratory; ²University of California, Riverside; ³Iowa

State University



9:25 AM Invited Microstructural Changes in Nanotwinned Metals under Various Deformation **Modes**: Andrea Hodge¹; ¹University of Southern California

9:55 AM

Effect of Cryogenic Equal Channel Angular Pressing on Mechanical Behavior and Microstructure of Pure Copper: Pedro Henrique Oliveira¹; Danielle Magalhães¹; Andrea Kliauga¹; Vitor Sordi¹; ¹Federal University of São Carlos

10:15 AM

Influence of Deformation on Microstructure of Al4Si and Cu4Nb Alloys during Friction Stir Processing: A Multi-modal Microstructural Characterization Study: Julian D. Escobar¹; Bharat Gwalani¹; Matthew Olszta¹; Joshua Silverstein¹; Luciano Bergmann²; Jorge dos Santos²; Peter Staron²; Emad Maawad²; Benjamin Klusemann²; Suveen Mathaudhu²; Arun Devaraj¹; ¹Pacific Northwest National Laboratory; ²Helmholtz-Zentrum Geesthacht

10:30 AM Invited

Hierarchical Microstructure in Shear Bands of Pure Titanium: Xiaolong Ma¹; Dexin Zhao²; Dinakar Sagapuram²; *Kelvin Xie*²; ¹Pacific Northwest National Lab; ²Texas A&M University

SPECIAL TOPICS

Design and Manufacturing Approaches for the Next Generation of Sustainable Materials: The 2021 Student-led Symposium — Challenges in Sustainable **Materials: Novel Processing and Recycling**

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: Mary Dougherty, Colorado School of Mines; Christopher Finfrock, Colorado School of Mines; Brady McBride, Colorado School of Mines; Jaden Zymbaluk, Colorado School of Mines; Desmond Mills, Colorado School of Mines; Casey Gilliams, Colorado School Of Mines

Monday AM March 15, 2021

Session Chairs: Mary Dougherty, Colorado School of Mines; Christopher Finfrock, Colorado School of Mines; Casey Gilliams, Colorado School of Mines; Brady McBride, Colorado School of Mines; Desmond Mills, Colorado School of Mines; Jaden Zymbaluk, Colorado School of Mines

8:30 AM

Introductory Comments: Design and Manufacturing Approaches for the Next Generation of Sustainable Materials: The 2021 Student-led Symposium: *Christopher Finfrock*¹; ¹Colorado School of Mines

8:35 AM Invited **Research with a Sustainable Materials Science and Engineering Approach**: Bryan *Boudouris*¹; Lynnette Madsen¹; ¹National Science Foundation

8:55 AM Invited **Research Requirements for Sustainable Materials**: *Daniel Cooper*¹; ¹University of Michigan

9:15 AM Invited

TMS

Creating New Green Jobs Starts at the Product Design Stage: Justine Burt¹;



11:35 AM Invited

9:35 AM Invited Materials Innovations Towards Decarbonization of Industrial Processes: Elsa *Olivetti*¹; ¹Massachusetts Institute of Technology

9:55 AM Invited Genomic Computational Design: Materials for Sustainability: Gregory Olson¹; ¹Massachusetts Institute of Technology

10:15 AM Invited Additive Manufacturing of High Temperature Materials: New Alloys and Sustainability Considerations: Tresa Pollock¹; ¹University of California, Santa Barbara

10:35 AM Invited Challenges in Optimizing Structural Metamaterials: Brad Boyce¹; Anthony Garland¹; Benjamin White¹; Ryan Alberdi¹; ¹Sandia National Laboratories

10:55 AM Invited

Microstructural Development and Powder Feedstock Recyclability in Additive Manufacturing by Laser Powder Bed Fusion: Yongho Sohn¹; Sharon Park¹; Holden Hyer¹; Nathalia Diaz Vallejo¹; Thinh Huynh¹; Asif Mahmud¹; Kevin Graydon¹; Cameron Lucas¹; Nicolas Ayers¹; Abhishek Mehta¹; Le Zhou¹; ¹University of Central Florida

11:15 AM Invited Shaping a Sustainable World Together – Delivering Novelis' Commitment to Sustainability: James Fekete¹; ¹Novelis Global Research and Technology Center





Using Rapid Alloy Prototyping to Investigate the Effects of Increased Levels of **Residual Elements from Recycled Scrap on DP800 Steel**: *Caroline Norrish*¹; Carlos Llovo-Vidal²; Richard Underhill²; Cameron Pleydell-Pearce¹; Nicholas Lavery¹; ¹Swansea University, Bay Campus; ²Tata Steel Europe

ELECTRONIC MATERIALS

Electronic Packaging and Interconnections 2021 — Pb-free Solder Alloys I

Sponsored by: TMS Functional Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Mehran Maalekian, Mat-Tech; Christopher Gourlay, Imperial College London; Babak Arfaei, Ford Motor Company; Praveen Kumar, Indian Institute of Science; Sai Vadlamani, Intel Corporation; Kazuhiro Nogita, University of Queensland; David Yan, San Jose State University

Monday AM March 15, 2021

Session Chairs: Mehran Maalekian, Mat-Tech; Amir Hossein Nobari, 5NPlus

8:30 AM Invited Nucleation and Growth Kinetics of Sn Whiskers Under Applied Pressure: Eric *Chason*¹; Piyush Jagtap¹; Nupur Jain¹; Allan Bower¹; ¹Brown University

8:50 AM

Development of Near Room Temperature Solder Alloys and Soldering Processes in Microelectronics: *Shiqian Liu*¹; Stuart McDonald¹; Tetsuro Nishimura²; Kazuhiro Nogita¹; ¹University of Queensland; ²Nihon Superior Co., Ltd



Energy Technologies and CO2 Management — Session I

9:10 AM Invited

Comparison of Corrosion for Ni- and Co-based Surface Finishes: Albert T. Wu¹; Si-Wei Lin¹; Shu-Chi Ku²; Nico Li²; ¹National Central University; ²Taiwan Uyemura Co., Ltd

9:30 AM Invited **Microstructural Evolution in Low-temperature Pb-free Solders**: *Nikhilesh Chawla*¹; ¹Purdue University

9:50 AM

Tailoring BSn Grain Orientations in Electronic Interconnections via Manipulating **Textures of Interfacial Intermetallics**: *Zhaolong Ma*¹; Ce Li¹; Xingwang Cheng¹; Suyuan Yang¹; ¹Beijing Institute of Technology

10:10 AM

Reliability Evaluation of Ag Sinter-joining Die Attach under a Harsh Thermal Cycling Test: *Zheng Zhang*¹; Chuantong Chen¹; Suetake Aiji¹; Ming-Chun Hsieh¹; Iwaki Aya¹; Katsuaki Suganuma¹; ¹Osaka University/ISIR

10:30 AM

Modeling Effect of Copper Solute on Electromigration Induced Stress Generation in Al-based Interconnects: *Kieran Cavanagh*¹; Ping-Chuan Wang¹; ¹SUNY New Paltz

MOBILE-FRIEND



ONTENTS

AB

Π

Q

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals **Division, TMS: Energy Committee**

Program Organizers: Alafara Baba, University of Ilorin; Lei Zhang, University of Alaska Fairbanks; Donna Guillen, Idaho National Laboratory; Xiaobo Chen, RMIT University; John Howarter, Purdue University; Neale Neelameggham, IND LLC; Cong Wang, Northeastern University; Ziqi Sun, Queensland University of Technology; Hong Peng, University of Queensland; Yu Lin Zhong, Griffith University

March 15, 2021 Monday AM

ENERGY & ENVIRONMENT

Session Chairs: Alafara Baba, University of Ilorin; Lei Zhang, University of Alaska Fairbanks

8:30 AM

CO, Emission Calculation Model of Integrated Steel Works Based on Process Analysis: Xinchuang Li¹; *Hui Li*²; Weijian Tian²; Zhe Chen²; Hao Bai²; ¹China Metallurgical Industry Planning and Research Institute; ²University of Science and **Technology Beijing**

8:50 AM

In-situ Electrode Temperature Monitoring and Thermal Runaway Detection of Li-ion Pouch Cell: Bing Li¹; Mihit Parekh¹; Vilas Pol¹; Thomas Adams¹; James Fleetwood¹; *Casey Jones*; Vikas Tomar¹; ¹Purdue University

9:10 AM

Experimental Study on Dust Removal Performance of Dynamic Wave Scrubber for Smelting Flue Gas: Fang Dong¹; Yan Liu¹; Xiaolong Li¹; Guili Liu¹; Tingan Zhang¹; ¹Northeastern University



Monday AM March 15, 2021

9:30 AM

Homogenization of the Dense Composite Membranes for Carbon-dioxide Removal: Dragutin Nedeljkovic¹; ¹American University of the Middle East

9:50 AM

Hydrodynamics of Gas-liquid Two-phase Flow in Reverse Spray Washing Process: *Xiaolong Li*¹; Tingan Zhang¹; Yan Liu¹; Guili Liu¹; Fang Dong¹; ¹Northeastern University

10:10 AM

Influence of Coal Reactivity on Carbon Composite Briquette Reaction in Blast Furnace: *Huiqing Tang*¹; Zi Yu¹; Tao Rong¹; ¹University of Science and Technology Beijing

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Lightweight Materials & High Entropy Alloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St. Petersburg Polytechnic University

MONDAY AM





8:30 AM

Case Study: Implementation of FSW in the Colombian Rail Transport Sector: *Elizabeth Hoyos*¹; Jeroen De Backer²; Santiago Escobar¹; Jonathan Martin²; Mauricio Palacio³; ¹Universidad EIA; ²TWI; ³Metro de Medellín

8:50 AM

Three Sheet Al Alloy Assembly for Automotive Application: *Piyush Upadhyay*¹; Hrishikesh Das¹; Daniel Graff¹; ¹Pacific Northwest National Laboratory

9:10 AM

Bobbin Friction Stir Processing of AZ31B Mg Alloy Plates: Eisha Khalid¹; Vasanth Shunmugasamy¹; *Bilal Mansoor*; ¹Texas A&M University at Qatar

9:30 AM

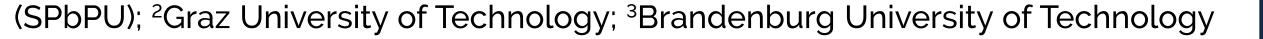
Characterization and Analysis of the Effective Wear Mechanisms on FSW Tools: *Michael Hasieber*¹; Michael Grätzel¹; Jean Pierre Bergmann¹; ¹Technische Universität Ilmenau

9:50 AM

Friction Stir Lap Welding between Aland FeCoCrNiMn High Entropy Alloy: Haining Yao¹; *Ke Chen*¹; Muyang Jiang¹; Min Wang¹; Xueming Hua¹; Lanting Zhang¹; Aidang Shan¹; ¹Shanghai Jiao Tong University

10:10 AM

Modified Friction Stir Welding of Al-Mg-Cu-Zn Aluminum Alloy: *Ahmad Alali Alkhalaf*¹; Anna Tesleva¹; Pavel Polyakov¹; Matthias Moschinger²; Sebastian Fritsche²; Iuliia Morozova³; Anton Naumov¹; Fedor Isupov¹; Gonçalo Pina Cipriano²; Sergio T. Amancio-Filho²; ¹Peter the Great St.Petersburg Polytechnic University



Cottbus-Senftenberg

10:30 AM Heterogeneous Structure-induced Strength-ductility Synergy by Partial Recrystallization during Friction Stir Welding of a High-entropy Alloy: Po-Ting Lin¹; *Hung-Chi Liu*¹; Po-Ying Hsieh¹; Cheng-Yu Wei¹; Che-Wei Tsai¹; Yutaka Sato²; Shih-Che Chen³; Hung-Wei Yen³; Nian-Hu Lu³; Chih-Hsuan Chen³; ¹National Tsing Hua University; ²Tohoku University; ³National Taiwan University

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Dendritic Growth

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials **Science and Engineering Committee**

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Monday AM March 15, 2021

Session Chairs: Charles-Andre Gandin, MINES ParisTech CEMEF UMR CNRS 7635; Damien Tourret, IMDEA Materials; Tomohiro Takaki, Kyoto Institute of Technology; Amy Clarke, Colorado School of Mines



MOBILE-FRIEND

8:30 AM

Introductory Comments: Frontiers in Solidification Science VIII: Damien Tourret¹; ¹IMDEA Materials

8:35 AM Invited

In-situ Measurement of Dendrite Tip Shape in a Metallic Alloy: Christoph Beckermann¹; H. Neumann-Heyme²; N. Shevchenko²; J. Grenzer²; S. Eckert²; ¹University of Iowa; ²Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

9:05 AM

Microstructural Evolution in Metallic Alloys during Solidification: *Tiberiu Stan*¹; Peter Voorhees¹; ¹Northwestern University

9:25 AM

Shapes of Dendritic Tips at Small and Large Undercoolings: Andrew Kao¹; Liubov Toropova²; Dmitri Alexandrov²; Peter Galenko³; ¹University of Greenwich; ²Ural Federation University; ³Friedrich Schiller University Jena

9:45 AM

A Model for Dendrite Fragmentation in Alloy Solidification: Hieram Neumann-*Heyme*¹; Kerstin Eckert¹; Christoph Beckermann²; ¹Helmholtz-Zentrum Dresden-Rossendorf (HZDR); ²University of Iowa

10:05 AM

Dendritic Spacing Selection during Al-Cu Casting: Experiments and Multiscale Simulations: Barbara Bellon¹; Ahmed Boukellal²; Thomas Isensee¹; John Coleman³; Matthew Krane³; Michael Titus³; Damien Tourret²; *Javier Llorca*⁴; ¹IMDEA Materials Institute & Polytechnic University of Madrid; ²IMDEA Materials Institute; ³Purdue University; ⁴IMDEA Materials Institute & Technical University of Madrid



10:25 AM

Characterization of Dendritic Spatially Extended 3D Patterns in Directional Solidification: Microgravity Experiments in DECLIC-DSI Onboard ISS and 3D Phase-field Simulations: Kaihua Ji¹; Fatima Mota²; Louise Strutzenberg³; Rohit Trivedi⁴; Nathalie Bergeon²; Alain Karma¹; ¹Northeastern University; ²Aix-Marseille Université; ³NASA Marshall Space Flight Center; ⁴Iowa State University

10:45 AM

Comparison of Solidification Characteristics of In-situ X-radiography Experiments and DNN Simulations: *Maike Becker*¹; Laszlo Sturz²; Dirk Bräuer¹; Florian Kargl¹; ¹German Aerospace Center (DLR); ²Access e.V.

11:05 AM

Grain Competition in Polycrystalline Columnar Dendritic Solidification: Scale Bridging between Phase Field and Cellular Automaton Methods: Elaheh Dorari¹; Kaihua Ji¹; Gildas Guillemot²; Charles-Andre Gandin²; Alain Karma¹; ¹Northeastern University; ²MINES ParisTech

11:25 AM

Interaction of Hydrogen-bubbles with the Approaching Solidification Front in Al-Cu Melt - An In-situ Study: Thomas Werner¹; Juliane Baumann¹; Maike Becker¹; Christoph Pickmann²; Laszlo Sturz²; Florian Kargl¹; ¹German Aerospace Center (DLR) - Institute of Materials Physics in Space; ²ACCESS e.V.

SPECIAL TOPICS

Frontiers of Materials Award Symposium: 2021 Functional Nanomaterials: Translating Innovation into Pioneering Technologies — Session I



Program Organizer: Huanyu Cheng, Pennsylvania State University

Monday AM March 15, 2021

8:30 AM

Introductory Comments: Frontiers of Materials Award Symposium: 2021 Functional Nanomaterials: Translating Innovation into Pioneering Technologies: *Huanyu Cheng*¹; ¹Pennsylvania State University

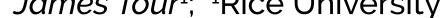
8:35 AM Invited Bio-inspired Artificial Vision and Wirelessly-integrated Wearable/Implantable **Device**: *Dae-Hyeong Kim*¹; ¹Seoul National University

9:15 AM Invited Graphene and 2D Materials for Wearable Electronic Devices and Biosensors: Jong-Hyun Ahn¹; ¹Yonsei University

9:55 AM Invited The Science of Contact-electrification and the Technology of Triboelectric **Nanogenerators**: *Zhong Wang*¹; ¹Beijing Institute of Nanoenergy and Nanosystems; Georgia Institute of Technology

10:35 AM Invited **Conformal Bioelectronic Interfaces**: *Xiaodong Chen*¹; ¹Nanyang Technological University

11:15 AM Invited Flash Joule Heating as a Rapid Solvent-free Scalable Route to New Materials: James Tour¹; ¹Rice University



NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Heterostructured Materials I: Fundamentals

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

March 15, 2021 Monday AM

Session Chairs: Cem Tasan, Massachusetts Institute of Technology; Jongun Moon, POSTECH; Yujie Wei, Institute of Mechanics, CAS; Deliang Zhang, Northeast University

8:30 AM Invited Gradients, Singularities and Interatomic Potentials: K. Parisis¹; Elias Aifantis¹; ¹Aristotle University of Thessaloniki

8:55 AM Invited and Localization Dependence of Strain Partitioning Microstructure in

Heterostructured Metals: C. Tasan¹; ¹Massachusetts Institute of Technology

9:20 AM Invited Nanoscale Heterogeneity and Gradients Engineered by Compositional Defect Decoration and Manipulation: The Atomic Scale Basis of Segregation Engineering: *Dierk Raabe*¹; ¹Max-Planck Institute

9:45 AM Invited Cu-FeBasedImmiscibleMedium-entropyAlloyswithExcellentTensileProperties: Jongun Moon¹; Jeong Min Park¹; Jae Wung Bae¹; Peter Liaw²; Hyoung Seop Kim¹; ¹POSTECH; ²The University of Tennessee

10:10 AM Invited Thickness-dependent Shear Localization in Cu/Nb Metallic Nanolayered **Composites**: *Caizhi Zhou*¹; Shujing Dong¹; ¹University of South Carolina

10:30 AM

Heterostructured Materials: An Emerging Materials Field with Great Potential: *Yuntian Zhu*¹; Xiaolei Wu²; Chongxiang Huang³; ¹North Carolina State University; ²Institute of Mechanics, CAS; ³Sichuan University

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Alloy **Development and Application I**



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Monday AM March 15, 2021

Session Chairs: Peter Liaw, The University of Tennesee; Carl Koch, North Carolina State Univ

8:30 AM Keynote Nanostructured High Entropy Alloys: A Review: *Carl Koch*¹; ¹North Carolina State University

9:00 AM Invited Exploring Benefits of Metastability in High Entropy Alloys: *C. Tasan*¹; Shaolou Wei¹; ¹Massachusetts Institute of Technology

9:25 AM Invited Opportunities and Trends in High Entropy Alloys: A Materials Science Perspective from the National Science Foundation: *Judith Yang*¹; ¹National Science Foundation

9:50 AM Invited Linking the Metallurgy of Multiple Principal Element Alloys to Properties: *David Shifler*¹; ¹Office of Naval Research

10:15 AM Invited Order and Disorder in Amorphous and High-entropy Alloys: Yong Zhang¹; *Xuehui Yan*²; ¹University of Science and Technology Beijing; ²University of Science and Technology Beijing

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling — Structures and Modeling I

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Monday AM March 15, 2021

Session Chairs: Chelsey Hargather, New Mexico Institute of Mining and Technology; Xie Xie, FCA US LLC

8:30 AM

Using Large Scale Ab Initio Computing to Predict and Understand High Entropy Alloys Formation: *Geoffroy Hautier*¹; Georgios Bokas¹; Wei Chen¹; Stéphane Gorsse²;

Antoine Hilhorst¹; Pascal Jacques¹; ¹Université catholique de Louvain; ²Institut de

Chimie de la Matière Condensée de Bordeaux

MONDAY AM

CONTENTS

TABLE

Q

8:50 AM

Mobility of Dislocations in FeNiCrCoCu High Entropy Alloys via Molecular **Dynamics Simulations**: *Yixi Shen*¹; Douglas Spearot¹; ¹University of Florida

9:10 AM Screening of Generalized Stacking Fault Energies, Surface Energies and Intrinsic **Ductile Potency of Refractory Multicomponent Alloys**: Yong-Jie Hu¹; Liang Qi¹; Aditya Sundar¹; ¹University of Michigan

9:30 AM Invited Efficient First-principles Methods of Calculating Stacking Fault Energies in High Entropy Alloys: Comparison of FCC and BCC Lattices: Joshua Strother¹; Alexandra Scheer¹; *Chelsey Hargather*¹; ¹New Mexico Institute of Mining and Technology

9:55 AM

Physics-based and Data-driven Micromechanics for Metastable High Entropy Alloys: Anssi Laukkanen¹; Matti Lindroos¹; Tatu Pinomaa¹; Tomi Suhonen¹; ¹VTT **Technical Research Center of Finland**

10:15 AM

Revisit the VEC Rule in High Entropy Alloys (HEAs) with High-throughput CALPHAD Approach and Its Applications for Material Design: A Case Study with Al-Co-Cr-Fe-Ni System: Songge Yang¹; Jun Lu¹; Fangzhou Xing²; Lijun Zhang²; Yu Zhong¹; ¹Worcester Polytechnic Institute; ²Central South University

MOBILE-FRIEND

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session I

Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

Monday AM March 15, 2021

Session Chair: Wei Xiong, University of Pittsburgh

8:30 AM

IntroductoryComments:Hume-RotherySymposium:AcceleratedMeasurements and Predictions of Thermodynamics and Kinetics for Materials Design and **Discovery**: *Wei Xiong*¹; ¹University of Pittsburgh

8:35 AM Keynote

William Hume-rothery Award Lecture: High-throughput Measurements of **Composition-dependent Properties of Alloy Phases for Accelerated Alloy Design**: *Ji-Cheng Zhao*¹; ¹University of Maryland

9:20 AM Invited **Combinatorial Design of High-entropy Alloys**: *Dierk Raabe*¹; Zhiming Li²; ¹Max-Planck Institute; ²Central South University

10:00 AM Invited **Emerging Capabilities for the High-throughput Characterization of Structural** Materials: Daniel Miracle¹; ¹Air Force Research Laboratory



MichaelKirka²; Ning Zhou³; Stephane Forsik³; *Tresa Pollock*¹; ¹University of California, Santa Barbara; ²Oak Ridge National Laboratory; ³Carpenter Technology Corp

Design of Cobalt Base Superalloys for 3D Printing: Sean Murray¹; Kira Pusch¹;

LIGHT METALS

11:20 AM Invited

Magnesium Technology 2021 — Keynote Session

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Petra Maier, University of Applied Sciences Stralsund; J. Brian Jordon, University of Alabama; Neale Neelameggham, IND LLC

March 15, 2021 Monday AM

Session Chairs: Victoria Miller, University of Florida; Petra Maier, Stralsund **University of Applied Sciences**

8:30 AM Keynote Measurement of the Critical Resolved Shear Stress for Slip in Mg Alloys Using Instrumented Indentation: *Warren Poole*¹; Shuheng Li¹; Ghazal Nayyeri¹; ¹University of British Columbia





9:15 AM Invited

Development of a Low-cost and Room-temperature Formable Mg Alloy Sheet with In-plane Isotropic Tensile Properties: Taiki Nakata¹; Chao Xu²; Hideaki Ohashi¹; Yu Yoshida³; Katsuhito Yoshida³; Shigeharu Kamado¹; ¹Nagaoka University of Technology; ²Harbin Institute of Technology; ³Sumitomo Electric Industries, Ltd.

9:45 AM Invited

Microstructure and Fracture Toughness of an Extruded Mg-Dy-Nd-Zn-Zr Alloy **Influenced by Heat Treatment**: *Petra Maier*¹; Benjamin Clausius¹; Charis Joy¹; Roman Menze²; Benjamin Bittner²; Norbert Hort³; ¹University of Applied Sciences Stralsund; ²Meko Laser Material Processing; ³Helmholtz-Zentrum Geesthacht

10:15 AM Invited

The High-solution Design of Magnesium Alloys: Yuan Yuan¹; Jun Wang¹; Xiongying Cheng¹; Tao Chen¹; Bin Jiang¹; Torben Boll²; Fushen Pan¹; ¹Chongqing University; ²Karlsruhe Institute of Technology

NUCLEAR MATERIALS

Materials and Chemistry for Molten Salt Systems — Corrosion

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short, Massachusetts Institute of Technology; Raluca Scarlat, University of California-Berkeley

TMS



8:30 AM

Introductory Comments: Materials and Chemistry for Molten Salt Systems: Stephen Raiman¹; ¹Texas A&M University

8:35 AM

Assessment and Qualification of Austenitic Stainless Steel for Use in Molten **Salts**: *George Young*¹; Micah Hackett¹; ¹Kairos Power

9:05 AM

Corrosion Behavior of SS316, Hastelloy X, and Hastelloy N in FLiNaK: Amanda Leong¹; Huali Wu¹; Jinsuo Zhang¹; ¹Virginia Tech

9:25 AM

Corrosion of 316 Stainless Steel in Molten Chloride Salt Micro Convection Loop: Yafei Wang¹; ¹University of Wisconsin Madison

9:45 AM

Development of an In-situ Mechanical Test System for Molten Salts: Jake Quincey¹; Peter Beck¹; Josef Parrington²; Lars Parrington²; Christopher Lamb²; George Young¹; Julie Tucker¹; Samuel Briggs¹; ¹Oregon State University; ²Parrington Instruments

10:05 AM

High-throughput Electrochemical Methods Development to Accelerate Molten Salt Corrosion-resistant Alloy Design: Bonita Goh¹; Yafei Wang¹; William Doniger¹; Phalgun Nelaturu¹; Dimitris Papailiopoulos¹; Dan Thoma¹; Kumar Sridharan¹; Adrien

Couet¹; ¹University Of Wisconsin Madison

10:25 AM Role of Alloy Chemistry in Governing Corrosion Rates of Candidate Materials for Molten Salt Reactors: Rishi Pillai¹; Cory Parker¹; Stephen Raiman¹; Bruce Pint¹; ¹Oak Ridge National Laboratory

10:45 AM

Influence of Corrosion Product Solubility and Dissimilar Materials on Corrosion of Alloys in Molten Salt Environment: Cody Falconer¹; William Doniger¹; Matthew Weinstein¹; Mohamed Elbakhshwan¹; Kumar Sridharan¹; Adrien Couet¹; ¹University of Wisconsin - Madison

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and **Beyond — Superalloys: Alloy Development**

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

March 15, 2021 Monday AM



MONDAY AM

TABLE OF

8:30 AM

Introductory Comments: Materials for High Temperature Applications-Next **Generation Superalloys and Beyond**: *Govindarajan Muralidharan*¹; ¹Oak Ridge National Laboratory

8:35 AM Keynote

Next Generation Superalloys and beyond for Aircraft Engine Applications: *Deborah Whitis*¹; ¹General Electric Co.

9:15 AM

CompositionallyGradedNanosizePrecipitatesatGrainBoundariesofDirectionally Solidified Nickel Based (GTD444) Superalloy: Richa Gupta¹; M.J.N.V. Prasad¹; Prita Pant¹; ¹IIT Bomaby

9:35 AM

TROPEA: A Platinum Containing New Generation Nickel-based Superalloy for Single Crystalline Applications: Jeremy Rame¹; Satoshi Utada²; Luciana Maria Bortoluci Ormastroni²; Lorena Mataveli Suave³; Edern Menou³; Lucille Després⁴; Paraskevas Kontis⁵; Jonathan Cormier⁶; ¹Safran Aircraft Engines; ²Institut Pprime -ISAE-ENSMA / Safran Aicraft Engines; ³Safran Tech; ⁴Institut Pprime - ISAE-ENSMA / Safran Tech; ⁵Max Planck Institut für Eisenforschung; ⁶Institut Pprime - ISAE-ENSMA

9:55 AM

Enhancing the Creep Performance of a Corrosion Resistant Ni-based Superalloy through Grain Boundary Design: Martin Detrois¹; Paul Jablonski¹; Jeffrey Hawk¹; ¹National Energy Technology Laboratory



Segregation-assisted Climb of Frank Partial Dislocations: A Novel Planar Fault Formation Mechanism in L12-hardened Superalloys: Malte Lenz¹; Erdmann Spiecker¹; Mingjian Wu¹; ¹Institute of Micro- and Nanostructure Research

10:35 AM

Microstructural Evolution under Complex Stress States during Creep of Single Crystal Ni-base Superalloy CMSX-4: Nicolas Karpstein¹; Malte Lenz¹; Jonathan Cormier²; Erdmann Spiecker¹; ¹Institute of Micro- and Nanostructure Research; ²Institut Pprime, CNRS-Université de Poitiers-ISAE ENSMA

10:55 AM Invited

On the Crack Growth Retardation under Dwell-fatigue in Nickel Disc Alloys: *Hangyue Li*¹; ¹University of Birmingham

11:25 AM

Crack Initiation Anisotropy of Ni-based Single-crystal Superalloys in the VHCF **Regime**: *Alice Cervellon*¹; Chris Torbet¹; Tresa Pollock¹; ¹University Of California Santa Barbara

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Processing Effects



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory

Monday AM March 15, 2021

8:30 AM Invited **Development of Modified 3Cr-3WVTa Base Bainitic Steels for Fusion Structural** Applications: Yukinori Yamamoto¹; Roger Miller¹; Arthur Rowcliffe¹; ¹Oak Ridge National Laboratory

9:00 AM

Low Temperature Neutron Irradiation and Mechanical Properties of Welded AISI **347**: Lauren Garrison¹; Nathan Reid¹; John Echols¹; Kaustubh Bawane¹; ¹Oak Ridge National Laboratory

9:20 AM

Neutron Irradiation Response of SA508 Pressure Vessel Steel Prepared by **Powder Metallurgy and Hot Isostatic Pressing**: *Yangyang Zhao*¹; Caleb Clement¹; Shujuan Wang²; Yaqiao Wu²; Katelyn Wheeler³; Donna Guillen³; David Gandy⁴; Janelle Wharry¹; ¹Purdue University; ²Boise State University, Center for Advanced Energy Studies; ³Idaho National Laboratory; ⁴Electric Power Research Institute



MOBILE-FRIENDL

9:40 AM

Dose and Temperature Dependence of Microstructure and Mechanical Properties in Ion-Irradiated PM-HIP Inconel 625: Caleb Clement¹; Janelle Wharry¹; Yangyang Zhao¹; David Gandy²; Shujuan Wang³; Yaqiao Wu³; ¹Purdue University; ²Electric Power Research Institute; ³Boise State University, Center for Advanced Energy **Studies**

10:00 AM Invited

Mechanical Behavior and Radiation Effect in Additively Manufactured 316L Stainless Steel: Meimei Li¹; Xuan Zhang¹; Wei-Ying Chen¹; ¹Argonne National Laboratory

10:30 AM

Mechanical Properties of Additively Manufactured 316L Stainless Steel before and after Neutron Irradiation: Thak Sang Byun¹; Timothy Lach¹; Maxim Gussev¹; Kurt Terrani¹; ¹Oak Ridge National Laboratory

10:50 AM **Effects of Low-temperature Neutron Irradiation and Post-weld Heat Treatment** on Tensile Properties of Welded Zircaloy-4: John Echols¹; Nate Reid¹; Sara Wonner¹; Lauren Garrison¹; ¹Oak Ridge National Laboratory

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ Experiments and Modeling — Session I



Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

Monday AM March 15, 2021

Session Chair: Minh-Son Pham, Imperial College

8:30 AM

In-situ X-Ray Diffraction Investigation of High-strain Rate, High-temperature Deformation in Microalloyed Steel: *Tim Wigger*¹; Rosa Pineda¹; Simon Hunt²; Danielle Fenech³; Ben Thomas⁴; Thomas Kwok⁵; David Dye⁵; Gorka Plata⁶; Jokin Lozares⁶; Inaki Hurtado⁶; Stefan Michalik⁷; Michael Preuss²; Mohammed Azeem⁸; Peter Lee¹; ¹University College of London; ²University of Manchester; ³University of Cambridge; ⁴University of Sheffield; ⁵Imperial College London; ⁶Mondragon Unibertsitatea; ⁷Diamond Light Source; ⁸University of Leicester

8:50 AM

In-situ Characterization of Material under Extreme Thermal Cycling Using Highspeed Synchrotron X-ray Diffraction: *Andrew Chuang*¹; Peter Kenesei¹; Yan Gao²; Jonathon Almer¹; Jun-Sang Park¹; ¹Argonne National Laboratory; ²GE Global

Research

9:10 AM

Mechanical Behavior and Microstructural Evolution of a Cu-0.7Cr-0.1Zr Alloy at Cryogenic Temperature: An In-situ Synchrotron X-ray Evaluation: *Pedro Henrique Oliveira*¹; Danielle Magalhães¹; Marcel Izumi²; Osvaldo Cintho²; Andrea Kliauga¹; Vitor Sordi¹; ¹Federal University Of São Carlos; ²State University Of Ponta Grossa

9:30 AM

A Quantitative Assessment of Stress / Strain Partitioning in a Dual-phase Titanium Alloy: Gaoming Zhu¹; *Shaolou Wei*; Cemal Tasan¹; ¹Massachusetts Institute of Technology

9:50 AM

Dislocation Density Inference from XRD Simulations of In-situ Microstructure Evolution Using Discrete Dislocation Dynamics: *Dylan Madisetti*¹; Jaafar El Awady¹; ¹Johns Hopkins University

10:10 AM Keynote

Microstructural Anisotropy and Its Influence on the Internal Stress Field within Grains: Experimental Confrontation with Full Field Crystal Plasticity Models: *Kaustubh Venkatraman*¹; Meriem Ben Haj Slama¹; Vincent Taupin¹; Nabila Maloufi¹; Stephane Berbenni¹; Anthony Rollett²; Martin Diehl³; Antoine Guitton¹; ¹Université de Lorraine – CNRS; ²Carnegie Mellon University; ³Max-Planck-Institut für Eisenforschung GmbH

10:50 AM

Impact of Precipitate Size, Orientation, and Temperature on Strain Hardening Behavior in Al-Cu Alloys: *Brian Milligan*¹; Dong Ma²; Lawrence Allard²; Amit Shyam²; Amy Clarke¹; ¹Colorado School of Mines; ²Oak Ridge National Laboratory



MONDAY AM

CONTENTS TABLE Q

Metal-Matrix Composites: Advances in Analysis, Measurement and **Observations – Metal Matrix Composites**

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Srivatsan Tirumalai, The University of Akron; William Harrigan, Gamma Alloys; Simona Hunyadi Murph, Savannah River National Laboratory

Monday AM March 15, 2021

Session Chair: Goswami Ramasis, Naval Research Laboratory

8:30 AM Invited The Mechanical Performance of an In Situ Processed Nickel-Titanium-Graphite Metal Matrix Composites: Influence of Processing: Amit Patil¹; Tushar Borkar¹; ¹Cleveland State University

9:00 AM

Development of Ultra-high Conductivity Metal Composites: *Keerti Kappagantula*¹; Xiao Li¹; Woongjo Choi¹; Glenn Grant¹; ¹Pacific Northwest National Laboratory

9:20 AM Invited Role of Microstructure on the Potential of MAX and MAB Phases and Their **Derivative-based Composites – A Review:** Surojit Gupta¹; ¹University of North Dakota

9:50 AM

Microstructure Evolution of Al/Ca Metal-Matrix Composite Conductor Wires by **Thermal Aging**: *Dustin Hickman*¹; Trevor Riedemann²; Iver Anderson²; ¹Iowa State University; ²Ames Laboratory

10:10 AM

Understanding the Mechanical Response of Friction Stir Welded In-situ Processed Aluminum Alloy Metal Matrix Composite: Experimental and Statistical Modelling **Approaches**: JimmyKarloopia¹; ShaikMozammil¹; PradeepJha¹; *SrivatsanTirumalai*²; ¹Indian Institute of Technology; ²University of Akron

10:40 AM

The Effect of Titanium Carbide and Spark Plasma Sintering Processing on Nickeltitanium Carbide Composites: Ganesh Walunj¹; Tushar Borkar¹; ¹Cleveland State University

11:00 AM

The Tribological Behavior of an In-situ Processed Magnesium Alloy Based Metal Matrix Composite: Arabinda Meher¹; Manas Mohan Mahapatra¹; ¹Indian Institute of Technology Bhubaneswar

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — Plenary



Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

March 15, 2021 Monday AM

8:30 AM Introductory Comments: Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt: Corby Anderson¹; ¹Colorado School of Mines

8:35 AM Introductory Comments: EPD Distinguished Lecture: Christina Meskers

8:40 AM Invited EPD Distinguished Lecture: Ferronickel - Thermodynamics, Chemistry, and **Economics**: *Rodney Jones*¹; ¹Mintek; University of the Witwatersrand; Pyro Consulting

9:10 AM Invited "Around the Nickel World in Eighty Days" A Virtual Tour of World Nickel Sulphide



MONDAY AM

and Laterite Operations and Technologies: *Phillip Mackey*¹; Ahmed Vahed¹; Tony Warner¹; ¹Worley

9:40 AM Invited A Review of Nickel Pyrometallurgy over the Past 50 Years with Special Reference to the Former INCO Ltd and Falconbridge Ltd.: A Vahed¹; Phillip Mackey¹; Anthony *Warner*¹; ¹Worley

10:10 AM Invited Establishing a Domestic Cobalt Supply Chain: Unlocking Challenging Feedstocks: *Frank Santaguida*¹; ¹First Cobalt Corporation

10:30 AM Invited Sustainable Developments in Nickel Recovery Process: John Quinn¹; Dennis Berger¹; *Shijie Wang*²; ¹Freeport McMoRan Mining; ²Rio Tinto Kennecott Utah **Copper Corp**

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Modeling and **Simulations**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Monday AM March 15, 2021

Session Chair: Fadi Abdeljawad, Clemson University

8:30 AM

Burgers Circuit Analysis of Grain Boundary Junctions: *Ian Winter*¹; Robert Rudd¹; Tomas Oppelstrup¹; Timofey Frolov¹; ¹Lawrence Livermore National Laboratory

8:50 AM

Electron-hole Carriers Induced Microstructure Evolution in Inorganic Semiconductors: Yidi Shen¹; *Qi An*¹; ¹University of Nevada, Reno

9:10 AM

Image-driven Discriminative and Generative Machine Learning Algorithms for Establishing Microstructure-processing Relationships: Wufei Ma¹; *Elizabeth Kautz*²; Arun Baskaran³; Aritra Chowdhury⁴; Vineet Joshi²; Bulent Yener³; Daniel Lewis³; ¹Purdue University; ²Pacific Northwest National Laboratory; ³Rensselaer Polytechnic Institute; ⁴GE Research Center



9:30 AM

Structure and Local Environment of Intermetallic Precipitate Phase Nucleus: *Deep Choudhuri*¹; ¹New Mexico Institute of Mining and Technology

9:50 AM

The Origin and Stability of Nanostructural Hierarchy in Nickel-base Superalloys: *Subhashish Meher*¹; Larry Aagesen¹; Tresa Pollock²; ¹Idaho National Laboratory; ²University of California Santa Barbara

10:10 AM

The Role of Grain Boundaries in Nanoscale Sintering: An Atomistic Simulation Study: Omar Hussein¹; Maher Alghalayini¹; *Fadi Abdeljawad*¹; ¹Clemson University

10:30 AM

A Phase Field Modeling Study on Coupling of Compositional Patterning with Evolution of Grain Boundaries in Irradiated Binary Immiscible Alloys: *Qun Li*¹; Pascal Bellon¹; Robert Averback¹; ¹University Of Illinois Urbana-Champain

10:50 AM

Characterizing Evolution of Grain Boundary Network Structure during Anisotropic Grain Growth.: *Jose Nino*¹; Oliver Johnson¹; ¹Brigham Young University

11:10 AM

Investigating the Microstructural Evolution of Cylindrical Interfaces: Anqi Qiu¹; Ian Chesser¹; Elizabeth Holm¹; ¹Carnegie Mellon University

MATERIALS PROCESSING

Phonons, Electrons and Dislons: Exploring the Relationships Between Plastic

TMS



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Aashish Rohatgi, Pacific Northwest National Laboratory; Sean Agnew, University of Virginia; Thomas Bieler, Michigan State University

Monday AM March 15, 2021

Session Chairs: Aashish Rohatgi, Pacific Northwest National Lab; Sean Agnew, University of Virginia; Thomas Bieler, Michigan State University

8:30 AM

Introductory Comments: Phonons, Electrons and Dislons: Exploring the **Relationships between Plastic Deformation and Heat**: *Aashish Rohatgi*¹; ¹Pacific Northwest National Laboratory

8:35 AM Invited Introduction to Dislons: A Quantized Description of Dislocations with Implications for Thermal and Electrical Transport: Mingda Li¹; ¹Massachusetts Institute of Technology

8:55 AM

Inelastic Neutron Scattering Investigation of the Phonon Spectra of Dislocated Nb Crystals: Sean Agnew¹; Thomas Bieler²; Matthew Stone³; ¹University of Virginia; ²Michigan State University; ³Oak Ridge National Laboratory

9:15 AM Invited

Dislocation-limited Thermal Transport in III-Nitride Materials: Lucas Lindsay¹; Hongkun Li²; Riley Hanus¹; Carlos Polanco¹; Andreas Zeidler³; Gregor Koblmuller³; Yee Kan Koh²; ¹Oak Ridge National Laboratory; ²National University of Singapore; ³Technical University of Munich

9:35 AM

Role of Tantalum Concentration and Processing Temperature on High Strain Rate Phonon Behavior in Copper-tantalum Alloys: Soundarya Srinivasan¹; Scott Turnage²; Billy Hornbuckle²; Chaitanya Kale¹; Kris Darling²; Kiran Solanki¹; ¹Arizona State University; ²Army Research Laboratory

9:55 AM Invited

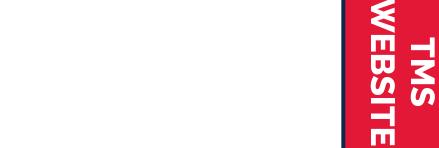
Dislocation Drag in Metals: Dependence on Velocity, Temperature, Density, and Crystal Geometry, and Its Effect on Material Response: Daniel Blaschke¹; Leonid Burakovsky¹; Abigail Hunter¹; Darby J. Luscher¹; Dean L. Preston¹; ¹Los Alamos National Laboratory

10:15 AM

The Effects of Heating Rate on Defect Reduction by Recrystallization in Deformed **Polycrystal Niobium**: *E. Nicometo*¹; Z. Thune¹; C. Edge¹; T. Bieler¹; ¹Michigan State University

NANOSTRUCTURED MATERIALS

Plasmonics in Nanocomposite Materials — From Theory to Application Session



Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Nasrin Hooshmand, Georgia Institute of Technology; Simona Hunyadi Murph, Savannah River National Laboratory; Mahmoud Abdelwahed, The University of Texas at San Antonio

Monday AM March 15, 2021

Session Chair: Nasrin Hooshmand, Georgia Institute of Technology

8:30 AM Keynote Gold and Au/Ni and Other Plasmonic Nanoparticles: Using Theory to Understand Metal Recovery and Optical Properties: *George Schatz*¹; ¹Northwestern University

9:15 AM Invited Anisotropic and Shape-selective Plasmonic Nanomaterials: Structure-property Relationships: *Simona Hunyadi Murph*¹; ¹Savannah River National Laboratory

9:45 AM Invited Nanophotonics for Neural Engineering: David Garfield¹; Emory Chan¹; Peter Schuck¹; Michel Maharbiz¹; *Maysam Chamanzar*²; ¹The Molecular Foundry, Lawrence Berkeley National Laboratory; ²Carnegie Mellon University

10:05 AM Invited Understanding Photocarrier and Gas Dynamics to Rationally Design Nanoheterostructured Photocatalysts for CO2 Conversion: Anthony Thompson¹; ¹Savannah River National Laboratory



MONDAY AM

CONTENTS

TABLE OF

ENERGY & ENVIRONMENT

Powder Materials for Energy Applications — Metal Powder Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee

Program Organizers: Kathy Lu, Virginia Polytechnic Institute and State University; Eugene Olevsky, San Diego State University; Hang Yu, Virginia Polytechnic Institute and State University; Ruigang Wang, The University of Alabama; Isabella Van Rooyen, Idaho National Laboratory

Monday AM March 15, 2021

Session Chairs: Hang Yu, Virginia Polytechnic Institute and State University; Ruigang Wang, The University of Alabama

8:30 AM

Introductory Comments: Powder Materials for Energy Applications: *Kathy Lu*¹; ¹Virginia Polytechnic Institute and State University

8:35 AM

Development of Gas Atomization Processes for Production of Passivated Calcium Powders: *Jordan Tiarks*¹; Dustin Hickman²; Trevor Riedemann¹; Iver Anderson¹; ¹Ames Laboratory; ²Iowa State University

8:55 AM

Utilizing Solid-state Grain Alignment to Bias Abnormal Grain Growth in

Strategically Designed Alnico Alloys: *Emily Rinko*¹; Timothy Prost²; Emma White³; Iver Anderson³; ¹Iowa State University; ²Ames Laboratory ; ³Ames Laboratory

8:30 AM Introductory Comments: Practical Tools for Integration and Analysis in Materials

9:15 AM Invited Wear Resistant Powder Materials for Energy Applications: Paul Prichard¹; Matthew Yao¹; ¹Kennametal Inc.

9:45 AM **ConformalCoating of Powders by Physical Vapor Deposition**: *Jonathan Priedeman*¹; Gregory Thompson¹; ¹University of Alabama

MATERIALS DESIGN

Practical Tools for Integration and Analysis in Materials Engineering — Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Titanium Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Adam Pilchak, US Air Force Research Laboratory; Michael Gram, Titanium Metals Corporation; William Joost; Raymundo Arroyave, Texas A&M University; Charles Ward, AFRL/RXM

Monday AM March 15, 2021

TABLE ONTENTS **Q**





MONDAY AM

Engineering: *Adam Pilchak*¹; ¹US Air Force Research Laboratory

8:35 AM Invited Accelerated Tools for Disordered-materials Discovery: Stefano Curtarolo¹; ¹Duke University

9:05 AM

Calculation of First Principles Based Thermodynamic and Kinetic Materials **Properties Using CASM**: *Brian Puchala*¹; John Thomas²; John Goiri²; Anton Van der Ven²; ¹University of Michigan; ²University of California, Santa Barbara

9:25 AM

A Framework for Closed-loop Materials Design Using Density Functional Theory: *Vinay Hegde*¹; Kevin Williams¹; Travis Ludlum¹; Maxwell Hutchinson¹; Eric Lundberg¹; Bryce Meredig¹; ¹Citrine Informatics

9:45 AM

Batch Reification Fusion Optimization (BAREFOOT) Framework: Richard *Couperthwaite*¹; Danial Khatamsaz¹; Abhilash Molkeri¹; Douglas Allaire¹; Ankit Srivastava¹; Raymundo Arroyave¹; ¹Texas A&M University

10:05 AM Invited

Microstructural Modeling with FiPy: *Jonathan Guyer*¹; Daniel Wheeler²; James Warren²; ¹National Institute of Standards & Technology; ²National Institute of Standards and Technology

10:35 AM

A Private Ledger Architecture Tailored for Secure Workflow Management in Additive Manufacturing Facilities: Evan Diewald¹; Jack Beuth¹; ¹Carnegie Mellon University



MOBILE-FRIEND

8:30 AM Introductory Comments: Rare Metal Extraction & Processing: Gisele Azimi¹; ¹University of Toronto

March 15, 2021 Monday AM

John Allison¹; ¹University of Michigan

MATERIALS PROCESSING

10:55 AM Invited

and Electrometallurgy Committee

Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The

Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan;

Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong

Rare Metal Extraction & Processing — Li, Co, Ni

11:25 AM The Materials Commons 2.0: A Collaboration Platform and Information Repository for the Global Materials Community: Brian Puchala¹; Glenn Tarcea¹; Tracy Berman¹;

LAMMPS as a Tool in Materials Modeling Workflows: Steve Plimpton¹; Aidan Thompson²; Mitch Wood²; ¹Sandia National Laboratories; ²Sandia National Labs



TABLE **ONTENTS** P

8:35 AM Keynote Scenarios of Future Lithium Use, 2021-2040: Roderick Eggert¹; ¹Colorado School of Mines

8:55 AM Invited The Importance of Spodumene Decrepitation on the Lithium Sulfate Extraction: Colin Dessemond¹; *Gervais Soucy*¹; ¹Université de Sherbrooke

9:15 AM

Application of Eutectic Freeze Crystallization in Recycling of Li-ion Batteries: *Yiqian Ma*¹; Michael Svärd¹; James Gardner¹; Richard Olsson¹; Kerstin Forsberg¹; ¹KTH - Royal Institute of Technology

9:35 AM Invited

Selective Separation of Co and Ni from REE in Recycling: Gulaim Seisenbaeva¹; Ani Vardanyan²; ¹Swedish University of Agricultural Sciences; ²Swedish University of Agricultural Sciences

9:55 AM

Recovery of Valuable Metals from End-of-life Lithium-ion Battery Using **Electrodialysis**: *Ka Ho Chan*¹; Monu Malik¹; Gisele Azimi¹; ¹University of Toronto

10:15 AM

Lithium Adsorption Mechanism for Li2TiO3: Raja Shekhar Marthi¹; York Smith¹; ¹University Of Utah

10:35 AM

Study on the Production of Lithium by Aluminothermic Reduction Method: Huimin Lu¹; Neale Neelameggham²; ¹Beihang University; ²IND LLC

10:55 AM Invited

Effect of Synthesis Method on the Electrochemical Performance of LiNixMnCo1x-yO2 (NMC) Cathode for Li-ion Batteries: A Review: Monu Malik¹; Ka Ho Chan¹;

LIGHT METALS

Sustainability in the Aluminum Supply Chain: Joint Session — Keynote Session

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Les Edwards, Rain Carbon Inc.

Monday AM March 15, 2021

Session Chair: Les Edwards, Rain Carbon Inc.

8:30 AM Introductory Comments: Sustainability in the Aluminum Supply Chain: Joint **Session**: Linus Perander; ¹

8:35 AM Introductory Comments: Sustainability in the Aluminum Supply Chain: Joint Session: Les Edwards¹; ¹Rain Carbon Inc.

8:40 AM Invited Long Term Sustainability of the Aluminium Sector: Pernelle Nunez¹; ¹International Aluminium Institute

9:05 AM Invited



Near Zero-waste and Near Break-even: A Path towards Sustainable Bauxite **Processing**: *Efthymios Balomenos*¹; ¹Mytilineos SA

9:30 AM Invited Alumina in a More Sustainable World: Andrew Furlong¹; ¹Worley

9:55 AM Invited **Review of Sustainability in the Carbon Supply Chain**: Les Edwards¹; ¹Rain Carbon Inc.

10:20 AM Invited Hydro's Approach to Sustainability: Hans Erik Vatne¹; ¹Hydro

10:45 AM Invited Aluminium Production: A Pathway to Zero Carbon by 2050: Mark Dorreen¹; ¹EnPot Limited

11:10 AM Invited The Aluminium Stewardship Initiative (ASI): Implementation and Impact: Fiona Solomon¹; *Marieke van der Mijn*¹; ¹Aluminium Stewardship Initiative

11:35 AM Question and Answer Period

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture and **Dislocations**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

March 15, 2021 Monday PM

Session Chair: Daniel Kiener, Montuniversität Leoben

2:00 PM Invited The Role of Fracture in the Reduction of Iron Ore with Hydrogen: Dierk Raabe¹; ¹Max-Planck Institute

2:40 PM Invited

Dislocation Pathways in Refractory Multi-principal Element Alloys: Fulin Wang¹; Glenn Balbus¹; Shuozhi Xu¹; Yanqing Su²; Jungho Shin¹; Paul Rottmann³; Keith Knipling⁴; Jean-Charles Stinville¹; Leah Mills¹; Oleg Senkov⁵; Irene Beyerlein¹; Tresa Pollock¹; *Daniel Gianola*¹; ¹University of California, Santa Barbara; ²Utah State University; ³University of Kentucky; ⁴U. S. Naval Research Laboratory; ⁵Air Force **Research Laboratory**

3:20 PM Invited

In Situ Observations and Measurements of Local Plastic Deformation and Fracture with 4D-STEM

: Yang Yang¹; Tom Pekin²; Ruopeng Zhang³; Shiteng Zhao³; Qin Yu¹; Sheng Yin¹; Colin Ophus¹; Mark Asta³; Robert Ritchie³; *Andrew Minor*³; ¹Lawrence Berkeley National Laboratory; ²Humbolt University, Berlin; ³University of California, Berkeley and Lawrence Berkeley National Laboratory



4:00 PM

Dislocations Processes in Fracture and Toughening Mechanisms of UFG bcc Metals at Room Temperature: Inas Issa¹; Anton Hohenwarter²; Jakub Zálešák¹; Daniel Kiener¹; ¹Montanuniversität Leoben, Austria; ²Montanuniversität Leoben, Austria.

4:20 PM

Imaging the Chemo-mechanical Coupled Fracture in Metal Passivation Layer by In-situ TEM: Yang Yang¹; Akihiro Kushima²; Huolin Xin³; Peter Hosemann⁴; Ju Li⁵; ¹Lawrence Berkeley National Laboratory; ²University of Central Florida; ³University of California, Irvine; ⁴University of California, Berkeley; ⁵Massachusetts Institute of Technology

SPECIAL TOPICS

2021 TMS Special Sessions – SMD/FMD Awards Ceremony & Special Lecture

Monday PM March 15, 2021

12:00 PM

FMD Awards Ceremony: Paul Ohodnicki¹; ¹University of Pittsburgh

12:15 PM

SMD Awards Ceremony & Introduction of Special Lecturer: Daniel Miracle¹; ¹Air

Force Research Laboratory

VEBSITE TMS

MOBILE-FRIEND

12:35 PM

SMD Special Lecturer: Pushing Structural Performance of Materials by Combining Alloy Design with Disruptive Manufacturing Technologies: Rajiv *Mishra*¹; ¹University of North Texas

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Titanium and Steel

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Monday PM March 15, 2021

Session Chair: John Lewandowski, Case Western Reserve University

2:00 PM Invited

Strain Accumulation during Fatigue and Fracture of Additively Manufactured Ti6Al4V: Experiments and Simulations: Raymundo Muro-Barrios¹; Raeann VanSickle¹; Huck Beng Chew¹; *John Lambros*¹; ¹University of Illinois



MONDAY PM

0

2:30 PM Effect of Defects on Stress State Dependent Fracture of Additively Manufactured **Metals**: *Allison Beese*¹; ¹Pennsylvania State University

2:50 PM

Structure-property Relationships to Explain the Elasto-plastic Anisotropy of Additively Manufactured Metal Alloys: Hunter Macdonald¹; Jishnu Battacharyya¹; Md Shamsujjoha¹; Sean Agnew¹; ¹University of Virginia

3:10 PM Invited

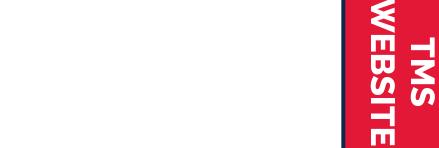
Design of Fatigue Resistant Additive Manufactured Austenitic Stainless Steels: Jonathan Pegues¹; Seungjong Lee²; Theron Rodgers¹; David Siaz¹; Shaun Whetten¹; Andrew Kustas¹; Michael Roach³; Nima Shamsaei²; ¹Sandia National Laboratories; ²Auburn University; ³University of Mississippi Medical Center

3:40 PM

Progressive Amplitude Fatigue Performance of Additively Manufactured Stainless Steel Superalloy: Sanna Siddiqui¹; Krystal Rivera¹; Isha Ruiz-Candelario¹; Ali Gordon²; ¹Florida Polytechnic University; ²University of Central Florida

ADDITIVE TECHNOLOGIES

Additive Manufacturing for Energy Applications III — Additive Manufacturing Processing



Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Nuclear Materials Committee

Program Organizers: Isabella Van Rooyen, Idaho National Laboratory; Indrajit Charit, University of Idaho; Subhashish Meher, Idaho National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Kumar Sridharan, University of Wisconsin-Madison; Xiaoyuan Lou, Auburn University

Monday PM March 15, 2021

Session Chair: Indrajit Charit, University of Idaho

2:00 PM Invited **Metal Additive Manufacturing for Energy Industries**: Edward Herderick¹; ¹Ohio State University

2:20 PM Invited Laser Powder Bed Fusion of Grade 300 Maraging Steel for Tooling Applications: Peeyush Nandwana¹; Rangasayee Kannan¹; Donovan Leonard¹; Derek Siddel¹; Chase Joslin¹; Ryan Dehoff¹; ¹Oak Ridge National Laboratory

2:40 PM

Additive Manufacturing of Zr-modified Aluminum Alloy 6061 by Laser-powder **Bed Fusion**: *Abhishek Mehta*¹; Le Zhou¹; Holden Hyer¹; Thinh Huynh¹; Sharon Park¹; Devin Imholte²; Nicolas Woolstenhulme²; Daniel Wachs²; Yongho Sohn¹; ¹University of Central Florida; ²Idaho National Laboratory

3:00 PM

MOBILE-FRIEND

Harnessing a High Energy, Superconducting Electron Beam for Additive and **Far-from-Equilibrium Manufacturing**: *Adam Duzik*¹; Justin Hill¹; ¹Mainstream **Engineering Corporation**

3:20 PM Invited

Novel Aspects of multi-Wire Arc Additive Manufacturing for Large Component Fabrication for Extreme Environments and New Alloy Discovery: Thomas Lillo¹; Nathan Huft¹; Denis Clark²; Michael Glazoff¹; Joel Simpson¹; ¹Idaho National Lab; ²DEClark Welding Engineering, PLLC

3:40 PM

Efficient Production of a High-performance Dispersion Strengthened, Multiprincipal Element Alloy: *Timothy Smith*¹; Aaron Thompson¹; Timothy Gabb¹; Christopher Kantzos¹; ¹NASA Glenn Research Center

4:00 PM

Investigation of the Effect of Laser Energy Density on Properties of Additively Manufactured Tungsten Lattices: Carly Romnes¹; Omar Mireles²; James Stubbins¹; ¹University of Illinois at Urbana-Champaign; ²NASA Marshall Space Flight Center

4:20 PM

Toward Part Qualification: Thermal Signature Analysis Using Wavelet Transform in Metal Additive Manufacturing: Sujana Chandrasekar¹; Jamie Coble¹; Amy Godfrey¹; Serena Beauchamp¹; Fred List²; Vincent Paquit²; Sudarsanam Babu¹; ¹University of Tennessee; ²Oak Ridge National Laboratory

4:40 PM

Effective Thermal Conductivity of Additively Manufactured Metal Matrix **Composite**: Saereh Mirzababaei¹; Venkata Vinay Krishna Doddapaneni¹; Kijoon Lee¹; Sriram Manoharan¹; Chih-hung Chang¹; Brian K. Paul¹; Somayeh Pasebani¹; ¹Oregon State University



Additive Manufacturing of Metals: Applications of Solidification Fundamentals - Micro-scale Modeling

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Solidification Committee

Program Organizers: Alex Plotkowski, Oak Ridge National Laboratory; Lang Yuan, University of South Carolina; Kevin Chaput, Northrop Grumman; Mohsen Asle Zaeem, Colorado School of Mines; Wenda Tan, University of Utah; Lianyi Chen, University of Wisconsin-Madison

Monday PM March 15, 2021

Session Chairs: Lianyi Chen, University of Wisconsin; Wenda Tan, University of Utah

2:00 PM

3D Analysis of Grain Morphologies and Solidification Texture in AM 316L: David *Rowenhorst*¹; ¹Naval Research Laboratory

2:20 PM

A Multi-scale Modeling Approach to Microstructure Prediction for Powder Bed Fusion Additive Manufacturing Processes Through Phase Field and Cellular Automata Methods: Daniel Dreelan¹; Abdur Rahman Al Azad¹; Alojz Ivankovic¹; Philip Cardiff¹; David Browne¹; ¹University College Dublin



2:40 PM

CA Model Sensitivity to Material Parameters, Nucleation, and Thermal Conditions Across AM Process Space: Matthew Rolchigo¹; Alex Plotkowski²; John Coleman²; Jim Belak¹; ¹Lawrence Livermore National Laboratory; ²Oak Ridge National Laboratory

3:00 PM

Controlling Additive Manufacturing Processes with Magnetic Fields: Andrew Kao¹; Teddy Gan¹; Xianqiang Fan²; Catherine Tonry¹; Ivars Krastins³; Peter Lee²; Koulis Pericleous¹; ¹University of Greenwich; ²UCL; ³University of Latvia

3:20 PM

Optimizing and Validating the Cellular Automata Finite Element Model for Additive Manufacturing: *Kirubel Teferra*¹; David Rowenhorst¹; ¹United States Naval Research Laboratory

3:40 PM

Prediction of Columnar-to-equiaxed Transition in Single Tracks during Laser Powder Bed Fusion Additive Manufacturing: Lang Yuan¹; Adrian Sabau²; David StJohn³; Arvind Prasad³; Peter Lee⁴; ¹University of South Carolina; ²Oak Ridge National Laboratory; ³The University of Queensland; ⁴University College London

4:00 PM

Effect of Kinetic Anisotropy on Microstructure Development during Simulated **Powder Bed Fusion of 316L Stainless Steel**: *Alexander Chadwick*¹; Peter Voorhees¹; ¹Northwestern University

4:20 PM

Microstructure Prediction Framework for Additively Manufactured Metals: Andrew Polonsky¹; Narendran Raghavan²; McLean Echlin³; Michael Kirka²; Ryan Dehoff²; Jonathan Madison¹; Tresa Pollock³; ¹Sandia National Laboratories; ²Oak Ridge National Laboratory; ³University of California, Santa Barbara



ADDITIVE TECHNOLOGIES



Additive Manufacturing: Materials Design and Alloy Development III -- Super Materials and Extreme Environments — Light Weight Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek Innovations LLC

March 15, 2021 Monday PM

Session Chair: Hunter Martin, HRL

2:00 PM Invited Architectured Interpenetrating Structures with Tailorable Energy Absorption in **Tension**: Zachary Cordero¹; ¹Massachusetts Institute of Technology

2:30 PM

Al-Cu-Zn-Mg Alloy for Additive Manufacturing by Electron Beam Deposition: Marcia Domack¹; *Cecilia Mulvaney*²; Christopher Domack³; Brandon Bodily⁴; Karen Taminger¹; ¹NASA Langley Research Center; ²University of Virginia; ³Analytical Mechanical Associates; ⁴Arconic Technology Center

2:50 PM

Development of High Strength and/or Corrosion-resistant Al Alloys with High **Printability**: *Le Zhou*¹; Holden Hyer²; Abhishek Mehta²; Sharon Park²; Thinh Huynh²; Brandon McWilliams³; Kyu Cho³; Yongho Sohn²; ¹Marquette University; ²University of Central Florida; ³CCDC Army Research Laboratory

3:10 PM

Ability of Creation of Aluminium Alloys with High Heat Conductivity Suitable for **3D Printing**: Mann Viktor¹; Krokhin leksandr¹; Vakhromov Roman²; Ryabov Dmitriy²; Mikhaylov Ivan²; *Kirill Nyaza*²; Grol Mariya²; ¹RUSSIAN Aluminum Management; ²Light Materials and Technologies Institute RUSAL Management

3:30 PM

High Strength WE43 Microlattices Manufactured by Laser Powder Bed Fusion: Holden Hyer¹; Qingyang Liu¹; Le Zhou¹; Dazhong Wu¹; Shutao Song¹; Yuanli Bai¹; Brandon McWilliams²; Kyu Cho²; *Yongho Sohn*¹; ¹University of Central Florida; ²CCDC Army Research Laboratory

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation – Session II**



Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Monday PM March 15, 2021

2:00 PM

3DMapsofGeometricallyNecessaryDislocationsinShock-loadedPolycrystalline **Tantalum**: *Wyatt Witzen*¹; Toby Francis¹; Tresa Pollock¹; Irene Beyerlein¹; ¹University of California Santa Barbara

2:20 PM

Dislocation Imaging by Precession Electron Diffraction: *Dexin Zhao*¹; Kelvin Xie¹; ¹Texas A&M University

2:40 PM

On the Mechanistic Origins of Maximum Strength in Nanocrystalline Materials: Ankit Gupta¹; Gregory Thompson²; Garritt Tucker¹; ¹Colorado School of Mines; ²University of Alabama

MOBILE-FRIEND

3:00 PM

Grain Boundary Slip Transfer Classification and Metric Selection with Artificial **Neural Networks**: *Zhuowen Zhao*¹; Thomas Bieler¹; Javier LLorca²; Philip Eisenlohr¹; ¹Michigan State University; ²IMDEA Materials Institute

3:20 PM

High Resolution Characterization of Dislocations Using Weak Beam Dark Field Scanning Transmission Electron Microscopy: *Jiashi Miao*¹; ¹Ohio State University

3:40 PM

Revisiting the Origin of Indentation Size Effect at Sub-micrometer Scales: *Xiaolong Ma*¹; Wesley Higgins²; Zhiyuan Liang²; Dexin Zhao²; George Pharr²; Kelvin Xie²; ¹Pacific Northwest National Laboratory; ²Texas A&M University

4:00 PM

Critical Resolved Shear Stresses (CRSS) of Hexagonal Titanium from Nanoindentation Optimization: Zhuowen Zhao¹; Mario Ruiz²; Jiawei Lu¹; Miguel Monclus²; Jon Molina-Aldareguia²; Thomas Bieler¹; Philip Eisenlohr¹; ¹Michigan State University; ²IMDEA Materials Institute

4:20 PM

Spatial Localization of Dislocation Avalanches in Microplasticity of a Highentropy Alloy: Quentin Rizzardi¹; Robert Maass¹; ¹University of Illinois at Urbana-Champaign

ADVANCED MATERIALS

Advanced High Strength Steels V – Session II



Sponsored by: TMS Structural Materials Division, TMS: Steels Committee

Program Organizers: Ana Luiza Araujo, CBMM North America Inc.; Louis Hector, General Motors Global Technical Center; Igor Vieira, Nucor Steel; Lijia Zhao, ArcelorMittal USA; Krista Limmer, CCDC Army Research Laboratory; Jonah Klemm-Toole, Colorado School of Mines; Sebastien Allain, Institut Jean Lamour; MingXin Huang, University of Hong Kong

Monday PM March 15, 2021

2:00 PM

Cryogenic Tensile and Microstructural Behaviors of High Manganese Steel Welds: *Myeonghwan Choi*¹; Junghoon Lee¹; Hyunbin Nam¹; Namhyun Kang¹; Myunghyun Kim¹; Daewon Cho²; ¹Pusan National University; ²Korea Institute of Machinery and **Materials**

2:20 PM

Effects of V and Mo Additions on the Suppression of HAZ Softening of Friction Stir Welded Si-Mn Martensitic Steel: Zexi Wu¹; Kohsaku Ushioda¹; Hidetoshi Fujii¹; ¹Joining and Welding Research Institute, Osaka University

2:40 PM

Microstructural Characterization of Fracture in Fe-10 pct Ni Gas Metal Arc Welds: *Richard Baumer*¹; Daniel Bechetti²; Matthew Sinfield²; ¹LeTourneau University; ²Naval Surface Warfare Center, Carderock Division

3:00 PM

Use of Physical Simulations for Accelerated Welding Procedure Development





in Supermartensitic Stainless Steels: Reed Phillips¹; Ezequiel Pessoa¹; *Richard Baumer*¹; ¹LeTourneau University

3:20 PM

Use of Thermo-mechanical Simulation to Assess Liquid Metal Embrittlement (LME) in Zinc Coated Advanced High Strength Steels: Kaleb Ponder¹; Dean Sage¹; Carolin Fink¹; Hassan Ghassemi-Armaki²; Michael Karagoulis³; *Antonio Ramirez*; ¹Ohio State University; ²ArcelorMittal Global R&D - East Chicago, East Chicago, IN, USA; ³Retired - General Motors

3:40 PM

Revisit the Slow Strain Rate Test for Hydrogen Embrittlement of Press-hardened **Steel**: Zuoheng Cao¹; *MingXin Huang*¹; ¹University of Hong Kong

4:00 PM

Methods for Improving the Hydrogen Embrittlement Resistance in Presshardened Steel: Zuoheng Cao¹; Xiaochuan Xiong²; *MingXin Huang*¹; ¹University of Hong Kong; ²Ironovation (Suzhou) Materials Technology

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII – Sustainability **Materials**



Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Monday PM March 15, 2021

Session Chairs: Surojit Gupta, University of North Dakota; Monu Malik, University of Toronto

2:00 PM

Design of Novel Agriculture-based Materials by Using Principles of Circular Economy: *Surojit Gupta*¹; ¹University of North Dakota

2:30 PM

Aluminum-ion Battery Made of AlCl₃-Trimethylamine Hydrochloride Ionic Liquid with Superior Performance: *Kok Long Ng*¹; Tony Dong¹; John Anawati¹; Gisele Azimi¹; ¹University of Toronto

2:50 PM

High Performing Vertically Aligned Graphene/Metal Oxide on Carbon Fiber Composite Electrodes for Wearable Supercapacitors and Strength Applications: Deepak Pandey¹; Kowsik Sambath Kumar¹; Jayan Thomas¹; ¹University of Central Florida



3:10 PM Investigation of Cost-effective AlCl3-urea Ionic Liquid Analog for Al-ion Batteries: *Monu Malik*¹; Kok Long Ng¹; Gisele Azimi¹; ¹University of Toronto

3:30 PM

Morphology Evolution and Interface Instability of Sodium Metal Electrodes: Susmita Sarkar¹; Partha Mukherjee¹; ¹Purdue University

CHARACTERIZATION

Advanced Real Time Imaging — Iron & Steelmaking

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

Monday PM March 15, 2021

Session Chairs: Il Sohn, Yonsei University; Jinichiro Nakano, USDOE National Energy Technology Laboratory



In-situ Real Time Observation of Austenite Formation in Duplex Stainless Steels during Different Cooling Conditions: Wangzhong Mu¹; Oscar Rova¹; Sohei Sukenaga²; Hiroyuki Shibata²; ¹Kth Royal Institute of Technology; ²IMRAM, Tohoku University

2:20 PM

Dissolution Mechanism of Oxide Particles in Silicate Melt: A Theoretical Study Supported by In-situ Observation Experiment: Changji Xuan¹; Wangzhong Mu²; ¹Sandvik Machining Solutions AB; ²Kth Royal Institute of Technology

2:40 PM

Direct Observation of Boron Nitride Dissolution in a Heat Resistant Martensitic Steel Using Confocal Scanning Laser Microscopy: Andrew (Drew) Huck¹; Bryan Webler¹; ¹Carnegie Mellon University

3:00 PM Invited **Observation of Surface and Interfacial Phenomena at High Temperature**: Masashi *Nakamoto*¹; ¹Osaka University

3:20 PM

Wetting and Spreading Kinetics between Liquid CaO-SiO2 Slags and a Solid SiO2: Chaeyeon Yoo¹; *Jaewoo Myung*¹; Yongsug Chung¹; ¹Korea Polytechnic University

3:40 PM

In-situ Quantitative Study of Heat Transfer Performance of Mold Flux by Using **Double Hot Thermocouple Technology**: *Zhe Wang*¹; Guanghua Wen¹; Wenbo Jiang¹; Ping Tang¹; Shuheng Huang¹; ¹Chongqing University



4:00 PM

In-situ Observation of Interfacial Phenomena between Magnetite and Matte at High Temperature by a Novel Optical Microscopic Technique: Seung-Hwan Shin¹; Sakiko Kawanishi¹; Sohei Sukenaga¹; Junichi Takahashi²; Hiroyuki Shibata¹; ¹Tohoku University; ²Sumitomo Metal Mining

BIOMATERIALS

Advances in Biomaterials for 3D Printing of Scaffolds and Tissues — Advances in Biomaterials for 3D Printing of Scaffolds and Tissues I

Sponsored by:

Program Organizers: Changxue Xu, Texas Tech University; Yifei Jin, University of Nevada, Reno; Zhengyi Zhang, Huazhong University of Science and Engineering; Jun Yin, Zhejiang University

Monday PM March 15, 2021

Session Chairs: Changxue Xu, Texas Tech University; Jun Yin, Zhejiang University

2:00 PM

A Bilayered GelMA/PEGDA-based Nerve Conduit with Supportive Cells for **Peripheral Nerve Regeneration**: *Jingyi Liu*¹; Yun Yin¹; ¹Zhejiang University

2:20 PM

A Novel Dual-layer Hydrogel/Cell Conduit Fabrication Method for Tissue **Engineering**: *Xixia Liu*¹; Jun Yin¹; ¹Zhejiang University



2:40 PM

Design and Evaluations System for 3D-printed Dental Implants Based on Deep Neural Networks: *Pei-Ching Kung*¹; Chai-Wei Hsu¹; An-Cheng Yang²; Nan-Yow Chen²; Nien-Ti Tsou¹; ¹National Chiao Tung University; ²National Center for Highperformance Computing

3:00 PM

Mechanical Properties and Biodegradability of Porous Mg and Zn Scaffolds Fabricated by Power Bed Laser Fusion for Biomedical Applications: Muzi Li¹; Felix Benn²; Thomas Derra²; Alexander Kopp²; Jon Molina-Aldareguía¹; Javier *Llorca*³; ¹IMDEA Materials Institute; ²Meotec; ³IMDEA Materials Institute & Technical University of Madrid

3:20 PM

Mechanical Properties and Biodegradability of Porous PLA/Mg and PLA/Zn Scaffolds Fabricated by Fused Filament Deposition for Biomedical Applications: Cristina Pascual¹; Cillian Thompson¹; Jimena de la Vega¹; De-Yi Wang¹; Carlos González²; Javier Llorca²; ¹IMDEA Materials Institute; ²IMDEA Materials Institute & **Technical University of Madrid**

3:40 PM

Laser-based Powder-bed Fusion Strategies for the Fabrication of Cellular Scaffolds with a Fine Resolution: Ebrahim Asadi¹; Fatemeh Hejripour¹; Md Abdus Salam¹; Faridreza Attarzadeh¹; Lauren Priddy²; Gary Bowlin¹; ¹University of Memphis; ²Mississippi State University

MOBILE-FRIEND

Advances in Powder and Ceramic Materials Science – Advanced Ceramics and Processes

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Materials Characterization Committee, TMS: Powder Materials Committee

Program Organizers: Bowen Li, Michigan Technological University; Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology; Kathy Lu, Virginia Polytechnic Institute and State University; Rajiv Soman, Eurofins EAG Materials Science LLC; Faqin Dong, Southwest University of Science and Technology; Jinhong Li, China University of Geosciences (Beijing); Ruigang Wang, The University of Alabama; Eugene Olevsky, San Diego State University

Monday PM March 15, 2021

Session Chairs: Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology

2:00 PM Invited Effect of Diamond Content and Modality on the Densification of Diamond Particulate Ceramic Composites by Hot-pressing: Jerry LaSalvia¹; Anthony DiGiovanni¹; Kristopher Behler¹; ¹CCDC Army Research Laboratory

2:25 PM

An Analysis on the Factors Affecting Oxidation Resistance of Silicon Containing Ultra High Temperature Borides Ceramics: Giuseppe Bianco Atria¹; Arvind Agarwal¹; Cheng Zhang¹; Ambreen Nisar¹; ¹Florida International University

TMS

MATERIALS DESIGN

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Al/Data Informatics: Applications and Uncertainty Quantification at Atomistics

March 15, 2021 **Monday PM**

and Mesoscales — Session II

Session Chairs: Vahid Attari, Texas A&M University; Wei Chen, Illinois Institute of Technology

2:00 PM

Uncertainty Quantification in Computational Thermodynamics - From the Atomistic to the Continuum Scale: Noah Paulson¹; Joshua Gabriel¹; Thien Duong¹; Marius Stan¹; ¹Argonne National Laboratory

2:30 PM

Bayesian Inference and Uncertainty Quantification of Grain Boundary Properties: Sterling Baird¹; Brandon Snow¹; Alexia Bigelow¹; David Fullwood¹; Eric Homer¹; Oliver Johnson; ¹Brigham Young University

2:50 PM

ZTEZIS

Q



MONDAY PM

A Bayesian Optimization Framework for Exploring the Grain Boundary Manifold: *Leila Khalili*¹; Owen Rettenmaier¹; Srikanth Patala¹; ¹North Carolina State University

3:10 PM

Machine Learning for Predicting Grain Boundary Properties: Lingxiao Mu¹; Elizabeth Holm¹; ¹Carnegie Mellon University

3:30 PM

Machine Learning Prediction of Defect Formation Energies: Vinit Sharma¹; Pankaj Kumar²; Pratibha Dev²; Ghanshyam Pilania³; ¹University of Tennessee Knoxville; ²Howard University; ³Los Alamos National Laboratory

3:50 PM

Accuracy, Uncertainty, Inspectability: The Benefits of Compositionally-restricted Attention-based Networks: Taylor Sparks¹; Steven Kauwe¹; Ryan Murdock¹; Anthony Wang²; ¹University of Utah; ²Technische Universitat Berlin

4:10 PM

A Probabilistic Approach with Built-in Uncertainty Quantification for the Calibration of a Superelastic Constitutive Model from Full-field Strain Data: Harshad Paranjape¹; Kenneth Aycock²; Craig Bonsignore¹; Jason Weaver²; Brent Craven²; Thomas Duerig¹; ¹Confluent Medical; ²U.S. Food and Drug Administration

4:30 PM

Uncertainty Quantification of Microstructures with a New Technique: Shape Moment Invariants: Arulmurugan Senthilnathan¹; Pinar Acar¹; ¹Virginia Tech

4:50 PM

Predicting Adsorption Energies and Surface Pourbaix Diagram of Metal NPs by **GCNN Method**: Kihoon Bang¹; Youngtae Park¹; Donghun Kim²; Sang Soo Han²; Hyuck Mo Lee¹; ¹KAIST; ²KIST



MATERIALS DESIGN



TABLE NTENTS **P**

Algorithm Development in Materials Science and Engineering — Machine Learning Algorithms and Computational Modeling for Study and Design **Materials**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Monday PM March 15, 2021

Session Chairs: Bryan Wong, University of California, Riverside; Bryce Meredig, **Citrine Informatics**

2:00 PM Invited Multi-Information Source Bayesian Optimization Applied to Materials Design: *RaymundoArroyave*¹; DanialKhatamsaz¹; RichardCouperthwaite¹; AbhilashMolkeri¹; Douglass Allaire¹; Ankit Srivastava¹; ¹Texas A&M University

2:30 PM

Understanding Grain Boundary Metastability Using the SOAP Descriptor and

Unsupervised Machine Learning Techniques: Lydia Serafin¹; Derek Hensley¹; Jay Spendlove¹; Gus Hart¹; Eric Homer¹; ¹Brigham Young University

2:50 PM

Grain Boundary Network Optimization through Human Computation and Machine **Learning**: *Christopher Adair*¹; Oliver Johnson¹; ¹Brigham Young University

3:10 PM Invited Deep Learning for Characterization of Deformation Induced Damage: Ulrich *Kerzel*¹; Setareh Medghalchi²; Carl Kusche²; Talal Al-Samman²; Sandra Korte-Kerzel²; ¹IUBH; ²RWTH Aachen University

3:40 PM

Automatic Segmentation of Microstructures in Steel Using Machine Learning Methods: Hoheok Kim¹; Junya Inoue¹; Tadashi Kasuya¹; ¹The University of Tokyo

4:00 PM

2D Microstructure Reconstruction for SEM via Non-local Patch-based Image Inpainting: Anh Tran¹; Hoang Tran²; ¹Sandia National Laboratories; ²Oak Ridge National Laboratory

4:20 PM Invited

Al-assisted Analysis of Flame Stability: Marius Stan¹; Jessica Pan²; Noah Paulson¹; Joseph Libera¹; ¹Argonne National Laboratory; ²Princeton University

4:50 PM

Neural Network Model of He Diffusion in W-based High Entropy Alloys: Gustavo Esteban-Manzanares¹; Enrique Martínez²; Duc Nguyen²; *Javier Llorca*³; ¹IMDEA Materials Institute; ²Los Alamos National Laboratory; ³IMDEA Materials Institute & Technical University of Madrid



2:00 PM Invited Challenges and Opportunities of Flexible Thermoelectric Devices Based on

5:10 PM

Comparison of Correction Schemes for Charged Point Defects in 2D Materials: *Preston Vargas*¹; Anne Marie Tan¹; Biswas Rijal¹; Richard Hennig¹; ¹University of Florida

ELECTRONIC MATERIALS

Alloys and Compounds for Thermoelectric and Solar Cell Applications IX — Session II

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Hsin-Jay Wu, National Chiao Tung University; Sinn-wen Chen, National Tsing Hua University; Franck Gascoin, Cnrs Crismat Unicaen; Philippe Jund, Montpellier University; Yoshisato Kimura, Tokyo Institute of Technology; Lan Li, Boise State University; Takao Mori, National Institute for Materials Science; Tiejun Zhu, Zhejiang University; Alexandra Zevalkink, Michigan State University; Wan-Ting Chiu, Tokyo Institute of Technology

Monday PM March 15, 2021

Session Chairs: Yi-Fen Tsai, National Chiao Tung University; Wan-Ting Yen, National Chiao Tung University

TABLE OF



Printing Technology: *Chien-Neng Liao*¹; ¹National Tsing Hua University

2:20 PM Invited Comparing Thermoelectricity of Bulk and Thin Film Heusler Alloys: *Ernst Bauer*¹; B. Hinterleitner¹; A. Riss¹; M. Parzer¹; F. Garmroudi¹; T. Mori²; X. Chen³; ¹Technische Universität Wien; ²NIMS; ³Shenyang National Laboratory for Materials Science

2:40 PM

Optimizing Thermoelectric Properties of Few-layer Transition Metal Dichalcogenides: *Tianhui Zhu*¹; Mona Zebarjadi¹; ¹University of Virginia

3:00 PM

Solid-state thermionic Devices: Effect of Asymmetry on the Device Performance: *Md Golam Rosul*¹; Mona Zebarjadi¹; ¹University of Virginia

3:20 PM

Interfacial Reaction in Ag/Se, Ag/Te, Ag2Te/Se and Ag2Te/Se-30at.%Te Couples and Their Related Phase Diagram: *Yohanes Hutabalian*¹; Sinn-wen Chen¹; ¹National Tsing Hua University

3:40 PM

Thermoelectric Cell Setup for Heat Recovery in Industrial Chimneys: Manuela Castañeda Montoya¹; Andrés Amell Arrieta¹; *Henry Colorado*¹; ¹Universidad de Antioquia

4:OO PM Invited Impact of Surface Engineering in Silicon Film Thermoelectrics: *Masahiro Nomura*¹; ¹The University of Tokyo

4:20 PM Invited

Developing Thermoelectric Thin Films and Modules for IoT Energy Harvesting:

TMS

*Takao Mori*¹; ¹National Institute for Materials Science

4:40 PM Invited

Thermomagnetic Transport in 2D Layered Topological Materials: Mona Zebarjadi¹; Md. Sabbir Akhanda¹; Emad Rezaei¹; Md. Golam Rosul¹; Keivan Esfarjani¹; Albert Davydov²; Sergiy Krylyuk²; ¹University of Virginia; ²NIST

5:00 PM Invited Cu-Sn Based Thiospinel Compounds: Insight of Alternative Route for Developing **Thermoelectrics Thiospinel Compounds?**: *Cédric Bourgès*¹; ¹Nims

5:20 PM

First-principles Calculation of Nernst Coefficient and Magneto-Seebeck: Emad *Rezaei*¹; Md Sabbir Akhanda¹; Keivan Esfarjani¹; Mona Zebarjadi¹; ¹University of Virginia

LIGHT METALS

Alumina and Bauxite — Process Optimization and Bauxite Enrichment

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Anne Duncan, Hatch

Monday PM March 15, 2021

TENTS Q



MONDAY PM

2:05 PM Invited

Implementation of Digital Technologies in Alumina Refining: A Producer **Experience**: *Vladimir Golubev*¹; Dmitry Mayorov¹; Dmitry Chistyakov¹; Evgeniy Fomichev¹; Ilya Blednykh¹; Andrey Panov¹; ¹RUSAL Engineering and Technological Center

2:40 PM

The Application of Intelligent Control to Red Mud Settling and Washing in Alumina **Refinery**: Yuehua Jiang¹; *Jinlong Tian*; Zhengyong Zhang¹; ¹Shenyang Aluminium and Magnesium Engineering and Research Institute Co., Ltd

3:00 PM **Alumina Refinery Volume Control**: *Thiago Franco*¹; ¹CBA

LIGHT METALS

Aluminum Alloys, Processing and Characterization — Alloy and MMC **Development**

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Dimitry Sediako, University of British Columbia

Monday PM March 15, 2021

Session Chair: Dimitry Sediako, University of British Columbia

2:00 PM Introductory Comments: Aluminum Alloys, Processing and Characterization:

Dimitry Sediako¹; ¹University of British Columbia

- WEBSITE TMS



MONDAY PM

CONTENTS

TABLE

Q

2:05 PM Invited

Anodization Compatibility of Eutectic Aluminum-Cerium Alloys: Zachary Sims¹; David Weiss²; Hunter Henderson³; Orlando Rios⁴; Jiheon Jun⁵; Sur Debashish⁶; Max Wiener⁷; Ryan Ott⁸; Fanggiang Meng⁸; ¹University of Tennessee; ²Eck Industries; ³Lawrence Livermore National Laboratory; ⁴University of Tennessee Knoxville; ⁵Oak Ridge National Laboratory; ⁶University of Virginia; ⁷Auto Anodics; ⁸Ames Laboratory

2:35 PM

Al-Sm Alloys Under Far-from-Equilibrium Conditions: Can Okuyucu¹; Burçin Kaygusuz¹; Cemil Isiksaçan²; Onur Meydanoglu²; Amir Motallebzadeh³; Sezer Özerinç¹; Yunus Kalay¹; ¹Middle East Technical University; ²Assan; ³Koç University

2:55 PM

EffectofMinorAdditivestoAl-Zn-MgAlloysonWeldingandCorrosionPerformance for Building Constructions: Alexander Gradoboev¹; Dmitriy Ryabov¹; Viktor Mann²; Aleksandr Krokhin²; Roman Vakhromov¹; Anna Ivanova¹; Anton Legkikh¹; ¹Light Materials and Technology Institute LLC; ²RUSAL Management JSC

3:15 PM

Mechanism Behind Al/Cu Interface Reaction: The Kinetics and Diffusion of Cu in Forming Different Intermetallic Compounds: Yongqiong Ren¹; Jie Chen¹; *Bingge* Zhao²; ¹Yonggu Group Corporation Co., Ltd.; ²Shanghai University

3:35 PM

Phase Formation of Mo- and Cr-rich Compounds in an Al-Si Cast Alloy: Peer Decker¹; Jan Steglich¹; Anna-Lena Kauws¹; Andreas Kiefert¹; Luisa Marzoli¹; Marcel Rosefort¹; ¹Trimet Aluminium SE

3:55 PM

Understanding the Effect of Quench Delay and Alloy Chemistry on Various 6000 **Series Alloys Systems**

: David Shoemaker¹; *Robert Matuska*¹; ¹Kaiser Aluminum

4:15 PM

Effect of Heat Treatment on the Microstructure and Mechanical Properties of LB-PBF AlSi10Mg and Scalmalloy: Shaharyar Baig¹; Seyed Ghiaasiaan¹; Nima Shamsaei¹; ¹Auburn University

4:35 PM

Thermal Properties of Hybrid Al-Cu-Components Produced by Combining **Powder Pressing and Semi-solid Forming Strategies**: *Marco Speth*¹; Mathias Liewald¹; Kim Rouven Riedmueller¹; ¹University of Stuttgart, Institute for Metal Forming Technology

4:55 PM Question and Answer Period Dr. Dimitry Sediako

LIGHT METALS

Aluminum Reduction Technology — Cell Modernization (Modelling and Energy **Optimization**)

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Nadia Ahli, Emirates Global Aluminium; Nancy Holt, Hydro Aluminium AS

Monday PM March 15, 2021

Session Chairs: Jayson Tessier , ALCOA; Andre Schneider, HATCH

TABLE

P

ONTENTS

2:00 PM Introductory Comments: Aluminum Reduction Technology: Nadia Ahli¹; ¹Emirates **Global Aluminium**

2:05 PM

Mass Transport by Waves: Bath-metal Interface Deformation, Rafts Collision and Physical Model: Lovatiana Rakotondramanan¹; László Kiss¹; Sándor Poncsák¹; Renaud Santerre¹; Sebastien Guerard²; Jean-François Bilodeau²; Simon Richer¹; ¹Grips Universite Du Quebec A Chicoutimi; ²Rio Tinto

2:25 PM

Modeling Anode Current Pickup After Setting: Choon-Jie Wong¹; Yuchen Yao¹; Jie Bao¹; Maria Skyllas-Kazacos¹; Barry J. Welch¹; Ali Jassim²; ¹University of New South Wales: ²Emirates Global Aluminum

2:45 PM

Superconductor Busbars – High Benefits for Aluminium Plants: Wolfgang Reiser¹; Till Reek²; Carsten Räch³; Daniel Kreutzer³; ¹Vision Electric Super Conductors GmbH; ²Martin Iffert Consulting; ³University of Applied Sciences Kaiserslautern

3:05 PM

Coupled SPH-DEM to Simulate the Injection of a Powder into a Liquid with Heat Transfer and Phase Change: Thomas Roger¹; Laszlo Kiss¹; Kirk Fraser²; Sandor Poncsak³; Sébastien Guérard³; Jean Francois Bilodeau³; Guillaume Bonneau¹; ¹Universite Du Quebec A Chicoutimi; ²National Research Council Canada; ³Rio **Tinto Aluminium**



MOBILE-FRIEND

Individual Anode Current Monitoring during Aluminum Reduction Cell Power **Reduction**: *Yuchen Yao*¹; Jie Bao¹; Maria Skyllas-Kazacos¹; Barry Welch¹; Ali Jassim²; ¹University of New South Wales; ²Emirates Global Aluminum

3:45 PM Question and Answer Period

BIOMATERIALS

Bio-Nano Interfaces and Engineering Applications — Bio-Nano II

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Biomaterials Committee**

Program Organizers: Candan Tamerler, University of Kansas; Kalpana Katti, North Dakota State University; Hendrik Heinz, University of Colorado Boulder; Terry Lowe, Colorado School of Mines; Po-Yu Chen, National Tsing Hua University

Monday PM March 15, 2021

Session Chairs: Candan Tamerler, University of Kansas; Feride Sermin Utku, Yeditepe University

2:00 PM Invited Flexible-glass Like Coating onto PTFE Vascular Graft Material via Nonthermal **Plasma Process**: Vineeth Vijayan¹; Bernabe Tucker¹; Yogesh Vohra¹; *Vinoy Thomas*¹; ¹University of Alabama at Birmingham

2:30 PM

Detection of Limonene Using Graphene Field Effect Transistor Modified by Selfassembling Peptide: Honma Chishu¹; Yoshiaki Sugizaki²; Atsunobu Isobayashi²;

Yuhei Hayamizu¹; ¹Tokyo Tech; ²Toshiba Corporation

2:50 PM

Enhancing Electrochemical Detection of Choline Using Molecularly Imprinted **Polymer Electrode**: Sermin Utku¹; *Sevgul Bakay*²; Adil Denizli³; Inci Cilesiz⁴; ¹Yeditepe University Biomedical Engineering; ²Duzce University; ³Hacettepe University; ⁴Istanbul Technical University

3:20 PM

Developing Nanostructured Metals for Innovative Medical Implants with Improved Design and Biofunctionality: Ruslan Valiev¹; Evgeny Parfenov¹; Olga Kulyasova¹; ¹UFA State Aviation Technical University

3:40 PM Invited

The Mechanical Significance of Sublamellar Organization of Mineralized Collagen **Fibrils**: Sermin Utku¹; ¹Yeditepe University Biomedical Engineering

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Advanced **Microstructure Characterization**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East



Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

March 15, 2021 Monday PM

Session Chairs: John Carpenter, Los Alamos National Laboratory; Mingming Zhang, ArcelorMittal Global R&D

2:00 PM

A Comparison between ZnO Cauliflowers on Glass and Aluminum Substrates: Shadia Ikhmayies

2:20 PM

Plastic Behavior and Texture Anisotropy in Dynamically Loaded Tin: Veronica Anghel¹; Carl Trujillo¹; Ramon Martinez¹; George Gray III¹; ¹Los Alamos National Laboratory

2:40 PM

Effect of Misorientation Development Near Grain and Twin Boundaries in Pure Copper and Copper-aluminium Alloy: Sandhya Verma¹; Prita Pant¹; M P Gururajan¹; ¹Indian Institute of Technology Bombay

3:00 PM

Rapid Irradiation and Characterization of HT9: *Gabriella Bruno*¹; Kevin Field¹; Li He²; T.M. Kelsy Green¹; Todd Allen¹; ¹University of Michigan; ²University of Wisconsin-Madison

3:20 PM

TMS

The Influence of Alloying in Stabilizing a Faceted Grain Boundary Structure:

Jonathan Priedeman¹; Gregory Thompson¹; ¹University of Alabama

3:40 PM

Crystal Mosaicity and Local Alloy Chemistry of Low Angle Grain Boundaries in Ni-based Superalloys: *Felicitas Scholz*¹; Junyang He²; Oliver Horst¹; Pascal Thome¹; Gunther Eggeler¹; Baptiste Gault²; Jan Frenzel¹; ¹Ruhr-Universitat Bochum; ²Max-Planck-Institut für Eisenforschung GmbH

4:00 PM

Insights into the Formation of Al-Cu Intermetallic Compounds during the Solidliquid Reaction by High-resolution Transmission Electron Microscopy: Jie Chen¹; Yongqiong Ren¹; *Bingge Zhao*²; ¹Yonggu Group Corporation Co., Ltd.; ²Shanghai University

NUCLEAR MATERIALS

Characterization of Nuclear Materials and Fuels with Advanced X-ray and Neutron Techniques — X-ray Diffraction/Scattering II

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Nuclear Materials Committee

Program Organizers: Xuan Zhang, Argonne National Laboratory; Jonathan Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University; Joshua Kane, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory; J. Kennedy, Idaho National Laboratory; Arthur Motta, Pennsylvania State University



MONDAY PM

ZTENTS

9

Monday PM March 15, 2021

Session Chairs: Arthur Motta, The Pennsylvania State University; Xuan Zhang, Argonne National Laboratory

2:00 PM Invited

In-situ Investigation into The Stability of Hydride Phases in Zirconium: *Fei Long*¹; Nima Badr¹; Matthew Topping¹; Igor Cherubin¹; Jun-Sang Park²; Mark Daymond¹; ¹Queens University; ²Advanced Photon Source

2:30 PM

In-situ Synchrotron X-ray Diffraction Study on Tensile Deformation of Neutron Irradiated Fe-Cr-C Alloys: *Hoon Lee*¹; Xiang Liu²; Mark Warren³; Dominic Piedmont¹; Xuan Zhang⁴; Meimei Li⁴; Jeff Terry³; Jonathan Almer⁴; James Stubbins¹; ¹University of Illinois at Urbana-Champaign; ²Idaho National Laboratory; ³Illinois Institute of Technology; ⁴Argonne National Laboratory

2:50 PM

MicrostructuralCharacterizationoftheStressandStrainDeformationPartitioning Evolution in Tungsten Heavy Alloys: *David Sprouster*¹; M. E. Alam²; G. R. Odette²; L Snead¹; ¹Stony Brook University; ²UCSB

3:10 PM

Creep Behavior of Advanced Austenitic (Fe-25Ni-20Cr) Alloy 709 through Insitu Neutron Diffraction Characterization and Transmission Electron Microscopy Characterization: Yuchen Zhao¹; *Ryan Schoell*¹; Matthew Frost²; Djamel Kaoumi¹; ¹North Carolina State University; ²Oak Ridge National Laboratory

3:30 PM

Using In-situ Synchrotron X-ray Scattering to Determine the TTT Diagram of



²Los Alamos National Laboratory; ³Y-12 National Security Complex

CORROSION

Coatings and Surface Engineering for Environmental Protection III — **Protection from Environmental Degradation, Session II**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Arif Mubarok, PPG; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University; Mary Lyn Lim, PPG Industries; Raul Rebak, GE Global Research; Brian Okerberg, PPG Industries

March 15, 2021 **Monday PM**

2:00 PM

Designing Lubricant-impregnated Coatings to Reduce Corrosion and Hydrogen **Embrittlement**: *Sami Khan*¹; Kripa Varanasi¹; ¹Massachusetts Institute of Technology

2:20 PM

Effects of Heat Treatments, Current Density, and Electroless Ni Layer Thickness on Corrosion Performance of Trivalent Chromium Passivations on ZnNi Coatings: *Kevin Foster*¹; William Fahrenholtz²; Matthew O'Keefe²; James Claypool²; ¹Missouri University of Science & Technology; ²Missouri University of Science & Technology



2:40 PM

Electronic Structure Mechanisms to Explain the Onset of Cl-induced Localised Corrosion in Al₂O₃: *Aditya Sundar*¹; Ganlin Chen¹; Liang Qi¹; ¹University of Michigan

3:00 PM

Galvanic Corrosion Mitigation by Material and Coating Selection for AZ31B boltjoined with CFRP: Yong Chae Lim¹; Jiheon Jun¹; Charles Warren¹; Zhili Feng¹; ¹Oak **Ridge National Laboratory**

3:20 PM

Using Mechanical and Ion Polishing to Identify Structural and Chemical Defects for the Pitting Corrosion of a Compositionally Complex Steel: Mark Wischhusen¹; Carol Glover¹; John Scully¹; Sean Agnew¹; ¹University of Virginia

NUCLEAR MATERIALS

Composite Materials for Nuclear Applications – Metal Based Composites

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee, TMS: Nuclear Materials Committee

Program Organizers: Anne Campbell, Oak Ridge National Laboratory; Dong Liu, University of Bristol; Rick Ubic, Boise State University; Lauren Garrison, Oak Ridge National Laboratory; Peng Xu, Idaho National Laboratory; Johann (Hans) Riesch, Max Planck Institute for Plasma Physics

March 15, 2021 Monday PM

Session Chair: Rick Ubic, Boise State University



.

2:00 PM

A Novel Processing Route for ODS Steel by Liquid Metallurgy: Shiqi Zheng¹; Xiaochun Li¹; ¹UCLA

2:20 PM

Competition between Void Evolution and Amorphization In Radiation-tolerant Nanocrystalline Cu-10at%Ta Alloy: *Priyam Patki*¹; Wei-Ying Chen²; Janelle Wharry¹; ¹Purdue University; ²Argonne National Laboratory

2:40 PM

Enhanced Microstructural Stability of ARB-processed Cu/Nb Nanolayers Under Heavy Dose Ion Irradiation at Elevated Temperatures: *Madhavan Radhakrishnan*¹; Thomas Nizolek²; Mukesh Bachhav³; Yongqiang Wang²; Nathan Mara⁴; Osman Anderoglu¹; ¹University of New Mexico; ²Los Alamos National Laboratory; ³Idaho National Laboratory; ⁴University of Minnesota

3:00 PM

Evaluation and Irradiation of 14YWT Capacitive Discharge Resistance Welds: *Calvin Lear*¹; Benjamin Eftink¹; Hyosim Kim¹; Todd Steckley¹; Thomas Lienert²; Stuart Maloy¹; ¹Los Alamos National Laboratory; ²T.J. Lienert Consulting, LLC

3:20 PM

IrradiationInducedForcedChemicalMixingandLocalHardeninginMechanicallyprocessed Immiscible Zr/Nb Multilayers: *Madhavan Radhakrishnan*¹; Thomas Nizolek²; Daniel Savage³; Marko Knezevic³; Nan Li²; Yongqiang Wang²; Mukesh Bachhav⁴; Boopathy Kombaiah⁴; Nathan Mara⁵; Osman Anderoglu¹; ¹University of New Mexico; ²Los Alamos National Laboratory; ³University of New Hampshire; ⁴Idaho National Laboratory; ⁵University of Minnesota



MONDAY PM

TABLE

ę

ONTENTS

3:40 PM

Mechanical Strength of Explosion Welded Thin Stainless-steel Cladding on Carbon Steel: Nathan Reid¹; Lauren Garrison²; John Echols²; Kaustubh Bawane³; Jean Paul Allain⁴; ¹University of Illinois Urbana Champaign; ²Oak Ridge National Laboratory; ³Idaho National Laboratory; ⁴Pennsylvania State University

4:00 PM

Radiation Tolerance and Microstructural Changes of Nanocrystalline Cu-Ta Alloy to High Dose Self-ion Irradiation: *Soundarya Srinivasan*¹; Chaitanya Kale¹; Billy Hornbuckle²; Kris Darling²; Matthew Chancey³; Efrain Hernández-Rivera²; Yimeng Chen⁴; Thomas Koenig⁵; Yongqiang Wang³; Gregory Thompson⁵; Kiran Solanki¹; ¹Arizona State University; ²Army Research Laboratory; ³Los Alamos National Laboratory; ⁴CAMECA Instruments Inc; ⁵The University of Alabama

4:20 PM

Synthesis and Irradiation Response of Hetero FeCr - Fe₂O₃ Interfaces: *Benjamin Derby*¹; Jon Kevin Baldwin¹; Djamel Kaoumi²; Danny Edwards³; Daniel Schreiber³; Timothy Lach⁴; Blas Uberuaga¹; Nan Li¹; ¹Los Alamos National Laboratory; ²North Carolina State University; ³Pacific Northwest National Laboratory; ⁴Oak Ridge National Laboratory

4:40 PM

Understanding Defect Recovery and Accommodation and Their Implications on Mechanical Performance in Irradiated Nanocomposite Materials: *Michael Wurmshuber*¹; David Frazer²; Mehdi Balooch³; Inas Issa¹; Andrea Bachmaier⁴; Peter Hosemann³; Daniel Kiener¹; ¹Montanuniversitaet Leoben; ²Los Alamos National Laboratory; ³University of California, Berkeley; ⁴Erich Schmid Institute of Materials Science

Computational and Modeling Challenges in Metals and Alloys for Extreme

Environments — High Strain Rates and Irradiation Effects

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Jean-Briac le Graverend, Texas A&M University; Jaafar El-Awady, Johns Hopkins University; Giacomo Po, University of Miami; Beñat Gurrutxaga-Lerma, University of Birmingham

Monday PM March 15, 2021

Session Chairs: Giacomo Po, University of Miami; Laurent Capolungo, Los Alamos National Lab

2:00 PM

Investigation of Role of Interface Microstructure on the Shock Compression and Spall Failure Behavior of Nanoscale Cu/Ta Multiphase Metallic Materials: *Marco Echeverria*¹; Avinash Dongare¹; ¹University of Connecticut

2:20 PM

Modeling of Laser Interactions with BCC Metals Using a Hybrid Atomisticcontinuum Approach: *Ching Chen*¹; Avanish Mishra¹; Sergey Galitskiy¹; Avinash Dongare¹; ¹University of Connecticut

2:40 PM

Mesoscale Modeling of Deformation Behavior of Fe-based Microstructures at



MOBILE-FRIENDL

High Strain Rates and under Shock Loading Conditions: *Ke Ma*¹; Avinash Dongare¹; ¹University of Connecticut

3:00 PM

The Microscopic Structure of a Heavily Irradiated Metal: *Peter Derlet*¹; Sergei Dudarev²; ¹Paul Scherrer Insitute; ²UKAEA CCFE

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics — Diffusion, Kinetics and Nonequilbrium Events

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

Monday PM March 15, 2021

Session Chairs: Pascal Bellon, University of Illinois at Urbana-Champaign; Enrique Martinez Saez, Clemson University; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Maylise Nastar, C.E.A

2:00 PM

Hydrogen Diffusion and Trapping in Multiphase Materials: A Multiscale Model for Non-point Trapping: *Fernando León-Cázares*¹; Dominic Dziedzic¹; Enrique GalindoNava¹; ¹University of Cambridge

2:20 PM

Kinetic Assessment of HCP Mg-Li-Al Alloys: *David Christianson*¹; Lilong Zhu²; Michele Manuel¹; ¹University of Florida; ²Yantai University

2:40 PM

Quantitative Inference of the Mobility Coefficient in the Cahn-Hilliard Equation from a Model Experiment: *Zirui Mao*¹; Michael Demkowicz¹; ¹Texas A&M University

3:00 PM Invited Defect Kinetics in Multi-component Oxides via Accelerated Molecular Dynamics: Blas Uberuaga¹; Ghanshyam Pilania¹; ¹Los Alamos National Laboratory

3:30 PM Invited Predicting Non-equilibrium Patterns Beyond Thermodynamic Concepts: **Application to Radiation Induced Microstructures**: *David Simeone*¹; Philippe Garcia¹; Laurence Luneville¹; ¹CEA

4:00 PM

Quantitative Phase-field Modeling for Corrosion of Engine Materials at High Temperature: Xueyang Wu¹; Michael Tonks¹; ¹University of Florida

4:20 PM Invited Molecular Dynamics Modeling of Embrittlement in Irradiated Nickel-base Alloys: *Michael Demkowicz*¹; ¹Texas A&M University

4:50 PM Invited

ONTENTS



MOBILE-FRIEND

Modeling Delayed-onset Kinetics of Materials Used in Nuclear Power Applications Using Atomistic Simulations: Laurent Béland¹; Cong Dai²; Peyman Saidi¹; Eric Nicholson³; Yu Luo¹; Chandra Singh³; Mark Daymond¹; Zhongwen Yao¹; ¹Queen's University; ²Canadian Nuclear Laboratories; ³University of Toronto

PHYSICAL METALLURGY

Continuous Phase Transformations — Session II

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee

Program Organizers: Jessica Krogstad, University of Illinois at Urbana-Champaign; Gregory Thompson, University of Alabama; Matthew Steiner, University of Cincinnati; Janelle Wharry, Purdue University

Monday PM March 15, 2021

Session Chairs: Janelle Wharry, Purdue University; Matthew Steiner, University of Cincinnati

2:00 PM Invited Effect of Bulk and Local Phase Transformation on Deformation Mechanisms: *Maryam Ghazisaeidi*¹; Mulaine Shih¹; Edwin Antillon²; ¹Ohio State University; ²Naval **Research Lab**

2:30 PM

Cross-Slip and Work-Hardening in Short-Range Ordered FCC Alloys: Anas Abu-

Odeh¹; Mark Asta¹; ¹University of California, Berkeley

- TMS WEBSITE

MONDAY PM

TABLE **ONTENTS P**

2:50 PM Invited

Structural Transformations Driven by Irradiation in the High Defect Density Limit: Sergei Dudarev¹; Daniel Mason¹; Peter Derlet²; ¹UK Atomic Energy Authority; ²Paul **Scherrer Institut**

3:20 PM

Magnetically Driven Short-range Order in the CrCoNi System: Flynn Walsh¹; Robert Ritchie¹; Mark Asta¹; ¹Lawrence Berkeley National Laboratory

3:40 PM

Short-range Clustering and Ordering Evolution of Ni-22Cr-13Mo Alloy: Po-Cheng *Kung*¹; Jessica Krogstad¹; ¹University of Illinois at Urbana-Champaign

4:00 PM

Thermodynamics of the Invar Transition: Phonons vs. Magnetism: Stefan Lohaus¹; Pedro Guzman¹; Brent Fultz¹; ¹California Institute of Technology

4:20 PM Invited Intrinsic Phase Stability and Continuous Phase Transformations in TiAlZrN Ultrahard Nitride Coatings: Vahid Attari¹; Raymundo Arroyave¹; ¹Texas A&M University

CORROSION

Corrosion in Heavy Liquid Metals for Energy Systems – Materials Compatibility with Liquid Metal Coolants II

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Nuclear Materials Committee

Program Organizers: Osman Anderoglu, University of New Mexico; Alessandro Marino, SCK-CEN; Michael Short, Massachusetts Institute of Technology; Peter Hosemann, University of California; Mike Ickes, Westinghouse Electric Company

Monday PM March 15, 2021

Session Chairs: Peter Hosemann, UC Berkeley; Michael Ickes, Westinghouse Electric Co.

2:00 PM

Numerical Modelling of Coolant Chemistry in Lead Bismuth Eutectic Cooled **Nuclear Reactors**: *Alessandro Marino*¹; Kristof Gladinez¹; Borja Gonzalez Prieto¹; Jun Lim¹; Kris Rosseel¹; Alexander Aerts¹; ¹SCK-CEN

2:20 PM Invited Behaviour of Spallation, Activation and Fission Products in LBE: Alexander Aerts¹; Borja Gonzalez Prieto¹; Jörg Neuhausen²; ¹SCK CEN; ²Paul Scherrer Institut

2:45 PM

Engineering Model of the Kinetics of the Steel Oxide Layer in a Flow of a Heavy Liquid Metal Coolant Under Various Oxygen Conditions: Alexander Avdeenkov¹; Alexander Orlov²; *Nafees Kabir*³; ¹«All-Russian Research Institute for Nuclear Power Plants Operation» JSC; ²Proryv JSC; ³MEPhI

3:05 PM Invited

Progress in LBE Chemistry Control and Measurement Techniques for MYRRHA: Jun Lim¹; Kristof Gladinez¹; Borja Gonzalez-Prieto¹; Alessandro Marino¹; Kris Rosseel¹; Alexander Aerts¹; ¹SCK CEN



3:30 PM

PILLAR: Pool-type Integral Leading Facility for Lead-alloy Cooled Advanced Small Modular Reactor, and Its Use for Natural Convection Study and Corrosion: Jaewon Choi¹; SangBum KIM¹; Kyunghwan Keum¹; Youho Lee¹; Il Soon Hwang²; Han-Chil Lee³; ¹Seoul National University; ²Ulsan National Institute of Science and Engineering (UNIST); ³Moojin

3:50 PM

Materials Compatibility Testing with Molten Lead up to 700°C: Osman Anderoglu¹; Cemal Cakez¹; Shuprio Ghosh¹; Khaled Talaat¹; Madhavan Radhakarishnan¹; Keith Woloshun²; Cetin Unal²; Stuart Maloy²; Michael Ickes³; Paolo Ferroni³; ¹University of New Mexico; ²Los Alamos National Laboratory; ³Westinghouse Electric Company

4:10 PM

Anubis Multiphysics: A Neutronics-Thermal Hydraulics Coupling Platform for Flow Accelerated Corrosion Modeling in Reactor Conditions: Khaled Talaat¹; Osman Anderoglu¹; ¹The University of New Mexico

4:30 PM

Performance of Candidate Alloys at 500°C in Flowing Lead: Cemal Cakez¹; Shuprio Ghosh¹; Khaled Talaat¹; Keith Woloshun¹; Stuart Maloy²; Cetin Unal²; Michael Ickes³; Paolo Ferroni⁴; Osman Anderoglu¹; ¹University of New Mexico; ²Los Alamos National Lab; ³Westinghouse Electric Corporation ; ⁴Westinghouse Electric Corporation

CHARACTERIZATION

Data Science and Analytics for Materials Imaging and Quantification — Session II: Data-led Approaches for 3D Characterization & X-Ray Imaging

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Emine Gulsoy, Northwestern University; Charudatta Phatak, Argonne National Laboratory; Stephan Wagner-Conrad, Carl Zeiss Microscopy; Marcus Hanwell, Brookhaven National Laboratory; David Rowenhorst, Naval Research Laboratory; Tiberiu Stan, Northwestern University

Monday PM March 15, 2021

Session Chair: Charudatta Phatak, Argonne National Laboratory

2:00 PM

Convolutional neural network-assisted recognition of nanoscale L12 ordered structures in face-centred cubic alloys: Yue Li¹; Leigh Stephenson¹; Raabe Dierk¹; Baptiste Gault¹; ¹Max-Planck-Institut für Eisenforschung GmbH

2:20 PM

Deep Neural Network Facilitated Complex Imaging of Phase Domains: Longlong *Wu*¹; Pavol Juhas¹; Shinjae Yoo¹; Ian Robinsion¹; ¹Brookhaven National Lab

2:40 PM

Quantitative X-ray Fluorescence Nanotomography: Mingyuan Ge¹; Xiaojing Huang¹; Hanfei Yan¹; Wilson Chiu²; Kyle Brinkman³; Yong Chu¹; ¹Brookhaven National Laboratory; ²University of Connecticut; ³Clemson University

3:00 PM

Materials Characterization in 3D Using High Energy X-ray Diffraction Microscopy: Irradiated and Deformed Materials: Hemant Sharma¹; Peter Kenesei¹; Jun-Sang

Park¹; Zhengchun Liu¹; Jon Almer¹; ¹Argonne National Laboratory

3:20 PM

Understanding the Keyhole Dynamics in Laser Processing Using Time-resolved X-ray Imaging Coupled With Computer Vision and Data Analytics: Jongchan *Pyeon*¹; Joseph Aroh¹; Runbo Jiang¹; Andy Ramlatchan²; Benjamin Gould³; Anthony Rollett¹; ¹Carnegie Mellon University; ²NASA Langley Research Center; ³Argonne National Laboratory

3:40 PM Question and Answer Period

MATERIALS PROCESSING

Deformation Induced Microstructural Modification – Session II: In Situ Interrogation of Microstructural Evolution During Deformation

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside ; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

Monday PM March 15, 2021

Session Chair: Bharat Gwalani, Pacific Northwest National Laboratory



2:00 PM Invited

Probing Microstructural Evolution in Deformation with Electrons and X-rays: Anthony Rollett¹; Robert Suter¹; Rachel Lim¹; Matthew Wilkin¹; Yueheng Zhang¹; Patcharapit Promoppatum²; Carter Cocke³; Ashley Spear³; Ricardo Lebensohn⁴; Jerard Gordon¹; ¹Carnegie Mellon University; ²KMUTT; ³University of Utah; ⁴Los **Alamos National Laboratory**

2:30 PM

In Situ Analysis of Microstructural Evolution of Metallic Alloys under High Speed **Rotational Shear Deformation**: Arun Devaraj¹; Tingkun Liu¹; Bharat Gwalani¹; Matthew Olszta¹; changyong Park²; Stanislav Sinogeikin³; Cynthia Powell¹; Suveen Mathaudhu⁴; ¹Pacific Northwest National Laboratory; ²High pressure collaborative access team; ³DAC tools; ⁴University of California Riverside

2:50 PM Invited

Deformation at a Single Precipitate Using a Nanocube Model System: Wendy *Gu*¹; Mehrdad Kiani¹; Mitsu Murayama²; ¹Stanford University; ²Virginia Tech

3:20 PM

In-situ Analysis of Microscale Deformation and Fracture in Severely Deformed Polycrystalline Tungsten: Lara Draelos¹; Zachary Levin¹; Ankit Srivastava¹; ¹Texas A&M University

SPECIAL TOPICS

Design and Manufacturing Approaches for the Next Generation of Sustainable Materials: The 2021 Student-led Symposium — Materials for Energy **Production and Storage**



Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: Mary Dougherty, Colorado School of Mines; Christopher Finfrock, Colorado School of Mines; Brady McBride, Colorado School of Mines; Jaden Zymbaluk, Colorado School of Mines; Desmond Mills, Colorado School of Mines; Casey Gilliams, Colorado School Of Mines

Monday PM March 15, 2021

Session Chairs: Christopher Finfrock, Colorado School of Mines; Casey Gilliams, Colorado School of Mines; Brady McBride, Colorado School of Mines; Desmond Mills, Colorado School of Mines; Jaden Zymbaluk, Colorado School of Mines

2:00 PM Invited III-V Photovoltaic Substrate Reuse and Recycle Strategies for Reduced Cost and Improved Materials Utilization: Corinne Packard¹; ¹Colorado School of Mines

2:20 PM Invited Reducing CO2 Emissions Through Improvements in the Materials Science of **Fossil Fuels**: Jonah Erlebacher¹; Shashank Lakshman¹; Gina Greenidge¹; ¹Johns Hopkins University

2:40 PM Invited Lithium-ion Battery Recycling Research at the ReCell Center: Linda Gaines¹; Bryant Polzin¹; *Jeffrey Spangenberger*¹; ¹Argonne National Laboratory

3:00 PM Invited



MONDAY PM

TABLE

9

NTENTS

Stepwise Approach to Improving Lead Furnace Operation Through Pilot Scale Studies and Computational Modeling: Alexandra Anderson¹; Joseph Grogan¹; John Wagner²; Sandeep Alavandi³; David Cygan³; ¹Gopher Resource; ²Gas Technology Institute ; ³Gas Technology Institute

LIGHT METALS

Electrode Technology for Aluminum Production — Carbon Anode Production – Where is the Cutting Edge? – A Focus on 4.0 and the Future

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Derek Santangelo, Hatch

March 15, 2021 Monday PM

Session Chair: Antti Koulumies, Outotec

2:00 PM Introductory Comments: Electrode Technology for Aluminum Production: Derek Santangelo¹; ¹Hatch

2:05 PM Invited Digitalization in the Carbon Area as a Means to Improve Productivity: Antti *Koulumies*¹; Paul Merlin¹; Ana Maria Becerra¹; ¹Metso Outotec

2:25 PM Invited AMELIOS Suite or the Fives Digital Package for Carbon 4.0: Christophe Bouche¹; Xavier Genin¹; Sylvain Georgel¹; *Pierre Mahieu*¹; ¹Fives



2:45 PM

Development and Applications of the Four Points Probe (4PP) Electrical Resistivity **Measurements for Anode Process Optimization**: Julien Lauzon-Gauthier¹; John Secasan¹; ¹Alcoa Corporation

3:05 PM Invited The Readiness and Compatibility of a Modern Anode Handling and Cleaning System for Industry 4.0 Technologies: Kevin Williams¹; ¹Advanced Dynamics Corporation Ltd.

3:25 PM Break

3:40 PM Panel Discussion

ELECTRONIC MATERIALS

Electronic Packaging and Interconnections 2021 – 3D Microelectronic Packaging and Emerging Interconnects

Sponsored by: TMS Functional Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Mehran Maalekian, Mat-Tech; Christopher Gourlay, Imperial College London; Babak Arfaei, Ford Motor Company; Praveen Kumar, Indian Institute of Science; Sai Vadlamani, Intel Corporation; Kazuhiro Nogita, University of Queensland; David Yan, San Jose State University

Monday PM March 15, 2021

MONDAY PM





Session Chairs: Praveen Kumar, Indian Institute of Science; Nilesh Badwe, Intel Corp.

2:00 PM

Electromigration of Cu-Cu Bonds Fabricated by Instant Bonding Using <111>-oriented Nanotwinned Cu Microbumps: Kai-Cheng Shie¹; Po-Ning Hsu¹; Yu-Jin Li¹; King-Ning Tu¹; Chih Chen¹; ¹National Chiao Tung University

2:20 PM

Enhancement on the Bonding Strength of Instantly-bonded Cu-Cu Joints by **Post Annealing**: *Jia Juen Ong*¹; Chih Chen¹; King-Ning Tu¹; ¹National Chiao Tung University

2:40 PM

High Electromigration Resistance of Nanotwinned Cu Redistribution Lines for Fan-out Packaging: I-Hsin Tseng¹; Chih Chen¹; Benson Lin²; Chia-Cheng Chang²; ¹National Chiao Tung University; ²MediaTek Inc

3:00 PM

Investigation of Interdiffusion In Micro Solder Joint with a Fine Pitch Copper Pillar Subjected to Electromigration Stressing: Hossein Madanipour¹; Yi Ram Kim¹; Allison Osmanson¹; Mohsen Tajedini¹; Choong-Un Kim¹; ¹University of Texas at Arlington

3:20 PM

On the 3D Evolution of the Nanoporous Structure of Sintered Ag on a Cu Substrate During Isothermal Aging Observed by In-situ X-ray NanoTomography: Kokouvi *N'Tsouaglo*¹; Azdine Nait-Ali¹; Mikael Gueguen¹; Pascal Gadaud¹; Loic Signor¹; Juan Creus²; Marc Legros³; Yijin Liu⁴; Xavier Milhet¹; ¹Prime Institute CNRS ENSMA; ²LASIE Université La Rochelle; ³CEMES CNRS; ⁴SLAC-SSRL



3:40 PM

Low Temperature Cu Direct Bonding with (111)-oriented Nanotwinned Copper Films on Metal Substrates: Hung-Che Liu¹; Chih Chen¹; ¹National Chiao Tung Universality

4:00 PM

Effect of Annealing on Mechanical Properties of nt-Cu Lines in Fan-out Wafer Level Packaging: Wei-You Hsu¹; Yu-Jin Li¹; I-Hsin Tseng¹; Benson Tzu-Hung Lin²; Chia-Cheng Chang²; Chih Chen¹; ¹National Chiao Tung University; ²MediaTek Inc.

4:20 PM

Direct Bonding Process of (111) Nanotwinned Copper Thin Films: *Jing-Yi Zhong*¹; Yung-Ting Tai¹; Fan-Yi Ouyang¹; ¹National Tsing Hua University

ENERGY & ENVIRONMENT

Energy Technologies and CO2 Management — Session II

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals **Division, TMS: Energy Committee**

Program Organizers: Alafara Baba, University of Ilorin; Lei Zhang, University of Alaska Fairbanks; Donna Guillen, Idaho National Laboratory; Xiaobo Chen, RMIT University; John Howarter, Purdue University; Neale Neelameggham, IND LLC; Cong Wang, Northeastern University; Ziqi Sun, Queensland University of Technology; Hong Peng, University of Queensland; Yu Lin Zhong, Griffith University



MONDAY PM

Monday PM March 15, 2021

Session Chairs: Donna Guillen, Idaho National Laboratory; Neale Neelameggham, IND LLC

2:00 PM

Low Energy Mesoporous Silica Recovery from a Nigerian Kaolinite Ore for Industrial Value Additions: Alafara Baba¹; Abdullah Ibrahim¹; Dele Fapojuwo²; Kuranga Ayinla¹; Daud Olaoluwa¹; Sadisu Girigisu³; Mustapha Raji¹; Fausat Akanji⁴; Abdul Alabi⁵; ¹University of Ilorin; ²University of Johannesburg; ³University of Ilorin; Federal Polytechnic Offa; ⁴SHEDA, Abuja; ⁵Kwara State University

2:20 PM

Prediction Model of Converter Oxygen Consumption Based on Recursive Classification and Feature Selection: *Liu Zhang*¹; Zhong Zheng¹; Kaitian Zhang¹; Xinyue Shen¹; Yongzhou Wang¹; ¹Chongqing University

2:40 PM

ReductionBehaviorsofHematitetoMetallicIronbyHydrogenatLowTemperatures: *Kun He*¹; Zhong Zheng¹; Hongsheng Chen¹; Weiping Hao¹; ¹Chongqing University

3:00 PM

Simulation and Optimization of Defluorination and Desulfurization Processes of Aluminum Electrolysis Flue Gas: Xueke Li¹; Yan Liu¹; Xiaolong Li¹; Tingan Zhang¹; ¹Northeastern University

3:20 PM

The Influence of Hydrogen Injection on the Reduction Process in the Lower Part of Blast Furnace: A Thermodynamic Study: Zeji Tang¹; Zhong Zheng¹; Hongsheng Chen¹; Kun He¹; ¹Chongqing University



A Study of Numerical Modeling of Jet Heating Phenomenon in a Porous Media: Qingxuan Luo¹; *Yuchao Chen*¹; Armin Silaen¹; Chenn Zhou¹; ¹Purdue University Northwest

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — High Melting Temperature Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St. Petersburg Polytechnic University

Monday PM March 15, 2021

2:00 PM

Study of Residual Stress and Microstructure Changes in Friction Stir Processed Dual Phase 980 Grade Steel: *Koichi Taniguchi*¹; Yong Chae Lim²; Jeffery Bunn²; Zhili Feng²; ¹JFE Steel Corporation; ²Oak Ridge National Laboratory

2:20 PM

Advances in High Temperature FSW: Single Use Tools: Jonathan Martin¹; ¹TWI Ltd.



2:40 PM

Phosphorus Segregation and Its Effect on Properties in Friction Stir Welded High Phosphorus Weathering Steel: *Takumi Kawakubo*¹; Kohsaku Ushioda¹; Hidetoshi Fujii¹; ¹Joining and Welding Research Institute Osaka University

3:00 PM

Friction Stir Welding of Armor Grade Steels: Stan Hawkes¹; Rafael Giorjao¹; Martin McDonnell²; *Antonio Ramirez*¹; Alex Thiel³; Michael Eff⁴; ¹Ohio State University; ²US Army; ³Oshkosh Corp.; ⁴EWI

3:20 PM

Friction Stir Welding of NiTi Shape Memory Alloy: Parker West¹; Vasanth Shunmugasamy²; *Bilal Mansoor*; Ibrahim Karaman¹; ¹Texas A&M University; ²Texas A&M University at Qatar

3:40 PM

On the Development of Friction Stir Welding to Repair or Mitigate Chlorideinduced Corrosion in 304L Austenitic Stainless Steel: *Ben Sutton*¹; Gabriella Marino¹; Rafael Giorjao¹; Jayendran Srinivasan¹; Antonio Ramirez¹; Jenifer Locke¹; ¹Ohio State University

4:00 PM

Low-force Friction Surfacing for Crack Repair in 304L Stainless Steel: Hemant Agiwal¹; Hwasung Yeom¹; Kumar Sridharan¹; Kenneth Ross²; Frank Pfefferkorn¹; ¹University of Wisconsin-Madison; ²Pacific Northwest National Laboratory

4:20 PM

Evaluation of Residual Stresses in Isothermal Friction Stir Welded 304L Stainless SteelPlates: MadhumantiBhattacharyya¹; Thomas-GnaupelHerold²; Krishnan Raja¹; Jens Darsell³; Saumyadeep Jana³; *Indrajit Charit¹*; ¹University of Idaho; ²National

Institute of Standards and Technology; ³Pacific Northwest National Laboratory



Frontiers in Solidification Science VIII — Convection & Gravity

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Monday PM March 15, 2021

Session Chairs: Sven Eckert, Helmholtz-Zentrum Dresden-Rossendorf; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Christoph Beckermann, University of Iowa; Tiberiu Stan, Northwestern University

2:00 PM Invited Permeability Prediction of Dendritic Mushy Zone by Phase-field and Lattice Boltzmann Simulations: *Tomohiro Takaki*¹; ¹Kyoto Institute of Technology

2:30 PM

Multiscale Modeling of Alloy Dendritic Growth with Liquid Convection: *Thomas Isensee*¹; Damien Tourret²; ¹IMDEA Materials Institute & Polytechnic University of

Madrid; ²IMDEA Materials Institute

2:50 PM Invited

Coupling of Solidification Grain Structures with Heat and Mass Transfers: *Charles-Andre Gandin*¹; Vincent Maguin¹; Gildas Guillemot¹; Chengdan Xue¹; Michel Bellet¹; Romain Fleurisson¹; Yijian Wu¹; Orianne Senninger¹; ¹MINES ParisTech CEMEF UMR CNRS 7635

3:20 PM

Understanding the Role of Magnetic Fields on Freckle Formation during Solidification through In Situ Imaging: *Xianqiang Fan*¹; Natalia Shevchenko²; Samuel Clark¹; Sebastian Marussi¹; Saurabh Shah¹; Robert Atwood³; Sven Eckert²; Andrew Kao⁴; Peter Lee¹; ¹University College London; ²Helmholtz-Zentrum Dresden-Rossendorf; ³Diamond Light Source; ⁴University of Greenwich

3:40 PM Invited

Solidification and Fluid Convection - The Story of an Inseparable Couple: Sten Anders¹; Natalia Shevchenko¹; Andrew Kao²; *Sven Eckert*¹; ¹Helmholtz-Zentrum Dresden-Rossendorf; ²University of Greenwich

4:10 PM

Directional Solidification of Al-10wt.%Cu Alloy in Hypergravity: *Ali Jafarizadeh Koohbanani*¹; Sonja Steinbach¹; Florian Kargl¹; ¹German Aerospace Center, Institute of Materials Physics in Space

4:30 PM

A Comparison of Terrestrial and Microgravity Isothermal Equiaxed Alloy Solidification through Machine Learning, Multi-stage Thresholding and Subdendrite-based In Situ X-ray Video Processing: *Jonathan Mullen*¹; Mert Celikin¹; Pádraig Cunningham¹; David Browne¹; ¹University College Dublin

VEBSITI

TMS



Frontiers of Materials Award Symposium: 2021 Functional Nanomaterials: Translating Innovation into Pioneering Technologies — Session II

Program Organizer: Huanyu Cheng, Pennsylvania State University

March 15, 2021 Monday PM

2:00 PM Invited Becoming Sustainable, The New Frontier in Soft Electronics and Robotics: Martin *Kaltenbrunner*¹; ¹Johannes Kepler University Linz

2:40 PM Invited Organic Bioelectronics for the Precise Sensing, Delivery and Processing of Biosignals: Magnus Berggren¹; ¹Linköping University

3:20 PM Invited Nanomembrane Materials for Electronic "Soft-Wear" and Micro-Robotic "Hard-Ware": Oliver Schmidt¹; ¹Leibniz IFW Dresden; TU Chemnitz

4:00 PM Invited Electronics on the Brain: George Malliaras¹; ¹University of Cambridge

4:40 PM Invited **3D Printing Functional Materials & Devices**: *Michael McAlpine*¹; ¹University of Minnesota

TENTS



MOBILE-FRIEND

LIGHT METALS

Greater Than the Sum of Its Parts — Concurrent Alloy Design and Processing Science: An LMD Symposium Honoring Raymond Decker — Session I

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Eric Nyberg, Tungsten Heavy Powder & Parts; J. Brian Jordon, University of Alabama; Wilhelmus Sillekens, European Space Agency; Neale Neelameggham, IND LLC; Vineet Joshi, Pacific Northwest National Laboratory

March 15, 2021 Monday PM

Session Chair: Victoria Miller, University of Florida

2:00 PM Invited Nickel-base Alloys Development: Then and Now: Victoria Miller¹; Aziz Asphahani²; ¹University of Florida; ²QuesTek

2:30 PM Invited New Under the Sun: Robert Carnahan¹; Victoria Miller²; ¹Retired; ²University of Florida

3:00 PM Invited **Development of Biomaterials at NanoMAG from a Historical and Commercial Perspective**: Victoria Miller¹; *Stephen LeBeau*²; ¹University of Florida; ²nanoMAG LLC

3:30 PM

Enabling High Strength AA7xxx Sheet for Automotive Hot Stamping Applications:

AMicrostructural Perspective: *Atish Ray*¹; Tudor Piroteala¹; Rashmi Ranjan Mohanty¹;

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Heterostructured Materials II: Mechanical Properties

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

Monday PM March 15, 2021

Session Chairs: Mingxin Huang, The University of Hong Kong; Ruslan Valiev, Ufa Aviation Technical University; Xiaolong Ma, Pacific Northwest National Lab.

2:00 PM Invited Grain-boundary Delamination-induced Toughening in 2 GPa Deformed and **Partitioned Steel:** Li Liu¹; *MingXin Huang*¹; ¹University of Hong Kong



MOBILE-FRIEND

Enhanced Mechanical Properties in 3D Interface Metallic Multilayers: Justin *Cheng*¹; Jon Baldwin²; Nan Li²; Shuozhi Xu³; Irene Beyerlein³; Nathan Mara¹; ¹University of Minnesota Twin Cities; ²Los Alamos National Laboratory; ³University of California, Santa Barbara

2:45 PM

Enhanced Mechanical Properties of Interface-strengthened UFG Tungsten and **Tungsten-based Nanocomposites**: *Michael Wurmshuber*¹; Simon Doppermann¹; Markus Alfreider¹; Michael Burtscher¹; Daniel Kiener¹; ¹Montanuniversitaet Leoben

3:05 PM

Effect of Alloying Additions on the Strength of Confined Nanocrystalline Layers: Sevda Fathipour¹; Amir Motallebzadeh²; Özgür Duygulu³; *Sezer Ozerinc*¹; ¹Middle East Technical University; ²Koç University; ³TÜBITAK Marmara Research Center

3:25 PM Invited

Heterostructured Ultrafine-grained Metallic Materials with Enhanced Superplasticity and Superior Strength: Ruslan Valiev¹; Maxim Murashkin¹; Nguyen Chinh²; ¹UFA State Aviation Technical University; ²Eötvös Loránd University

3:50 PM Invited Hierarchical 3D Nanolayered Duplex-phase Zr with High Strength, Strain Hardening, and Ductility: Weizhong Han¹; ¹Xi'an Jiaotong University

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Alloy **Development and Application II**



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Monday PM March 15, 2021

Session Chairs: Veerle Keppens, Univ of Tennessee; Ke An, Oak Ridge National Laboratory

2:00 PM Invited Synthesis and Mechanical Properties of High Entropy Oxide Spinels: Veerle Keppens¹; Brianna Musico¹; Kurt Sickafus¹; Quinton Wright¹; Joshua Smith¹; ¹University of Tennessee

2:25 PM Invited Phase Formation, Structure Modulation and Property Optimization of High Entropy Alloys, Composites and Glasses: Jurgen Eckert¹; ¹Erich Schmid Institute of Materials Science

2:50 PM Invited High Etropy Alloy Design Aided by Neutron Scattering: Ke An¹; Rui Feng¹; Sichao Fu¹; ¹Oak Ridge National Laboratory

MONDAY PM



MOBILE-FRIEND

3:15 PM Invited

Combining Elemental and Microstructure Heterogeneities in High-entropy Alloys to Enhance Radiation Resistance: Yanwen Zhang¹; Miguel L. Crespillo²; Walker L. Boldman²; Philip D. Rack²; Hongbin Bei¹; Yongqin Chang³; Li Jiang⁴; Lumin Wang⁴; William J. Weber²; ¹Oak Ridge National Laboratory; ²University of Tennessee; ³University of Science and Technology Beijing; ⁴University of Michigan

3:40 PM

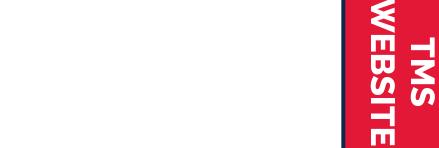
Distinctive Room Temperature Deformation Behavior in Plastic BCC Refractory High-entropy Alloys: Chanho Lee¹; Gian Song²; Michael Gao³; Wei Chen⁴; Ke An⁵; *Peter Liaw*¹; ¹University of Tennessee; ²Kongju National University; ³National Energy Technology Laboratory/Leidos Research Support Team; ⁴Illinois Institute of Technology; ⁵Oak Ridge National Laboratory

4:00 PM

Metastability and Phase Selection in High Entropy Alloys: Sebastian Kube¹; Pamela Banner¹; Sungwoo Sohn¹; David Uhl²; Amit Datye¹; Suchismita Sarker³; Apurva Mehta³; Jan Schroers¹; ¹Yale University; ²Southern Connecticut State University; ³SLAC National Accelerator Laboratory

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling - Structures and Modeling II



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Monday PM March 15, 2021

Session Chairs: Diana Farkas, Virginia Polytechnic Institute; Irene Beyerlein, University Of California, Santa Barbara

2:00 PM Invited

Mechanisms of Short-range Ordering and Cluster Formation and their Effects on Mechanical Properties of High-entropy Alloys: Shuai Chen¹; Zachary Aitken¹; Subrahmanyam Pattamatta²; Zhaoxuan Wu²; Zhi-Gen Yu¹; Rajarshi Banerjee³; David Srolovitz²; Peter Liaw⁴; *Yong-wei Zhang*¹; ¹Institute of High Performance Computing, A*STAR; ²City University of Hong Kong; ³University of North Texas; ⁴University of Tennessee

2:25 PM Invited

Development of Interatomic Potentials to Model the Deformation Behaviors in Highly Concentrated/Entropy-stabilized Ni-base Superalloys: *Ridwan Sakidja*¹; Andrew Duff²; Wai-Yim Ching³; Caizhi Zhou⁴; ¹Missouri State University; ²STFC; ³University of Missouri-Kansas City; ⁴University of South Carolina



2:50 PM Invited Structural Essentiality for Plasticity of High-entropy Alloys Profiled by Data Mining: Wei-Ren Chen¹; *Chi-Huan Tung*²; Shou-Yi Chang²; Yue Fan³; Zhitong Bai³; Changwoo Do¹; ¹Oak Ridge National Laboratory; ²National Tsing Hua University; ³University of Michigan

3:15 PM Invited Deformation Behavior of a Model High Entropy Alloy from Atomistic Simulations: *Diana Farkas*¹; ¹Virginia Polytechnic Institute

3:40 PM

Phase-Field Dislocation Dynamics Modeling of Refractory Multi-Principal Element Alloys: *Lauren Smith*¹; Abigail Hunter²; Irene Beyerlein¹; ¹University Of California, Santa Barbara; ²Los Alamos National Laboratory

4:00 PM

Statistics of the NiCoCr Medium-entropy Alloy: Novel Aspect of an Old Puzzle: *Zongrui Pei*¹; Rui Li²; G. Malcolm Stocks³; Michael Gao¹; ¹National Energy Technology Laboratory; ²University of Tennessee, Knoxville; ³Oak Ridge National Laboratory

4:20 PM

Phase Stability of NbVZrMx (M = Ti, Mo; x = 0 – 1) Refractory Complex Concentrated Alloys: *Zhaohan Zhang*¹; Mu Li¹; Guodong Ren¹; Arashdeep Thind¹; Katharine Flores¹; Rohan Mishra¹; ¹Washington University in St.Louis

4:40 PM

EAM and RF-MEAM Potentials for Thermal Properties of Zirconium Diboride: *Bikash Timalsina*¹; Alin Niraula¹; William Fahrenholtz²; Gregory Hilmas²; Andrew Duff³; Ridwan Sakidja¹; ¹Missouri State University; ²Missouri University of Science and Technology; ³Science and Technology Facilities Council

TMS /EBSITI

MATERIALS PROCESSING

High Temperature Electrochemistry IV — Session I

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Guy Fredrickson, Idaho National Laboratory

March 15, 2021 Monday PM

Session Chair: Uday Pal, Boston University, Boston, USA

2:00 PM

SelectiveExtractionofGoldfromGold-copperAlloyUsingAnodicElectrochemical **Deposition in Molten Salt Electrolyte**: *Takanari Ouchi*¹; Shuang Wu¹; Toru Okabe¹; ¹The University of Tokyo

2:30 PM

High-speed Electrodeposition of Textured Monolithic Lithiated Transition Metal Oxide Cathodes for Low Cost, High Energy, and Fast Charging Li-ion Batteries. John Cook¹; ¹Xerion Advanced Battery Corp

3:00 PM

Characterization of Uranium Electrodeposits Separated in Molten ClLiK Salt with Varied Applied Overpotentials and Uranium-cerium Compositions: Dimitris *Killinger*¹; Supathorn Phongikaroon¹; ¹Virginia Commonwealth University



3:30 PM Molten Hydroxide Mediated Electrosynthesis of Layered Transition Metal Oxides for Electrochemical Energy Storage: Arghya Patra¹; Paul Braun¹; ¹University of Illinois at Urbana-Champaign

MATERIALS DESIGN

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session II

Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

Monday PM March 15, 2021

Session Chair: Wei Chen, Illinois Institute of Technology

2:00 PM Invited

An Atom-Probe Tomogaphy Study of the Temporal Evolution of Concentration Retention Excesses and Depletions at gamma-f.c.c/gamma-prime-L12 Interfaces in a Ni-Al-Cr-Re Superalloy: David Seidman¹; ¹Northwestern University

2:40 PM Invited **Extended Applications of the CALPHAD Simulations**: Fan Zhang¹; Duchao Lv¹; Weisheng Cao¹; Shuanglin Chen¹; Chuan Zhang¹; Songmao Liang¹; ¹CompuTherm LLC



MONDAY PM

CONTENTS

TABLE

Q

3:20 PM Invited

Computational Modeling-assisted Development of Alumina-Cast forming Austenitic Stainless Steels for High Temperature Corrosive Environments: Govindarajan Muralidharan¹; Yukinori Yamamoto¹; Michael Brady¹; Shivakant Shukla¹; Tanya Ros²; Stanley Fauske³; Roman Pankiw⁴; Jim Myers⁵; ¹Oak Ridge National Laboratory; ²Arcelor Mittal Global R & D; ³Arcelor Mittal Coatesville; ⁴Duraloy Technologies; ⁵Metaltek International

4:00 PM Invited Visualizing and Rationalizing Synthesis Pathways in Oxides: Gerbrand Ceder¹; ¹University of California, Berkeley

4:40 PM Invited

High-throughput Testing and Characterization of Novel Additive Manufactured Materials: Madelyn Madrigal-Camacho¹; Adam Freund¹; Kendrick Mensink¹; Guillermo Aguilar¹; *Suveen Mathaudhu*¹; ¹University of California, Riverside

NUCLEAR MATERIALS

Materials and Chemistry for Molten Salt Systems – Corrosion & Chemistry

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short, Massachusetts Institute of Technology; Raluca Scarlat, University of California-

Berkeley

Monday PM March 15, 2021

Session Chair: Jinsuo Zhang, Virginia Tech

2:00 PM

Corrosion Control of 316H Stainless Steel and Nickel-Based Alloys in Molten Chloride Salts: Kasey Hanson¹; Krishna Moorthi Sankar¹; Remi Dingreville²; Joshua Sugar²; Chaitanya Deo¹; Preet Singh¹; ¹Georgia Institute of Technology; ²Sandia National Laboratories

2:20 PM

Analysis of Particulate Properties of Commercial FLiNaK in a 316 Stainless **Steel System.**: *Timothy Kennedy*¹; Timothy Head¹; NEXT Lab²; ¹Abilene Christian University; ²NEXT Lab

2:40 PM

Chemical Interaction Between Molten Flibe and Nitrate Solar Salt: Michael Hanson¹; Michael Zupan¹; Augustus Merwin¹; Francesco Carotti¹; Alan Kruizenga¹; ¹Kairos Power

3:00 PM

Mechanistic Understanding of 3D Morphological Evolution of Metals in Molten **Salts**

by In Situ X-ray Nano-tomography: Xiaoyang Liu¹; Arthur Ronne¹; Lin-Chieh Yu¹; Mingyuan Ge²; Lingfeng He³; Phillip Halstenberg⁴; Cheng-Hung Lin¹; Bobby Layne²; Sheng Dai⁴; Wah-Keat Lee²; Shannon Mahurin⁴; James Wishart²; Xianghui Xiao²; Yu-chen Karen Chen-Wiegart⁵; ¹Stony Brook University; ²Brookhaven National Laboratory; ³Idaho National Laboratory; ⁴Oak Ridge National Laboratory; ⁵Stony Brook University/Brookhaven National Laboratory

CONTENTS

TABLE

Q

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao,

3:20 PM

Effect of Impurities on Corrosion and Its Control in Molten FLiNaK: Krishna Moorthi Sankar¹; Preet Singh¹; ¹Georgia Institute of Technology

3:40 PM

Complex Structure of Molten NaCl-CrCl2 and NaCl-CrCl3: Cr-Cl Octahedra **Network and Intermediate-range Order**: *Boris Khaykovich*¹; Qing-Jie Li¹; David Sprouster²;Guiqiu(Tony)Zheng¹;JoergNeuefeind³;AlexBraatz³;JoannaMcFarlane³; Stephen Tsz Tang Lam¹; Daniel Olds⁴; Matthew Marshall⁵; Ju Li¹; ¹Massachusetts Institute of Technology; ²Stony Brook University; ³Oak Ridge National Laboratory; ⁴Brookhaven National Laboratory; ⁵Radiation Monitoring Devices

4:10 PM

Electrochemistry and Corrosion Studies for Alloy Development for Molten Salt Reactors (MSRs): *William Doniger*¹; Cody Falconer¹; Matthew Weinstein¹; Mohamed Elbakshwan¹; Govindarajan Muralidharan²; Adrien Couet³; Kumar Sridharan³; ¹University Of Wisconsin Madison; ²Oak Ridge National Laboratory; ³University of Wisconsin Madison

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Mineral and Material Processing

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee



MONDAY PM

University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology Company Ltd.; Shadia Ikhmayies

Monday PM March 15, 2021

Session Chairs: Baojun Zhao, University of Queensland; Yong Shi, Futianbao **Environment Technologies**

2:00 PM Keynote Materials Processing: From Ideas to Practice: Jiann-Yang Hwang¹; ¹Michigan Technological University

2:30 PM Invited

Recent Progress in Microwave-assisted Pyrometallurgy at Central South **University**: Liancheng Wang¹; *Zhiwei Peng*¹; Jie Wang¹; Wenxing Shang¹; Qiang Zhong¹; Mingjun Rao¹; Guanghui Li¹; Tao Jiang¹; ¹Central South University

2:50 PM Keynote **Production and High Ratio Application of Iron Ore Pellets in Shougang**: Gele Qing¹; Minge Zhao¹; Gang An¹; Kai Wang¹; xiaojiang Wu¹; zhixing Zhao¹; ¹Shougang Group

3:10 PM

Comparison between Compression Strength of Two Castor Oil Polyure than e Resin Matrix Composites Reinforced with Coconut or Piassava Fiber: Juliana Carvalho¹; Jessika Azevedo¹; Noan Simonassi²; *Felipe Lopes*³; Carlos Vieira¹; ¹Universidade Estadual do Norte Fluminense; ²State University of Northern Rio de Janeiro; ³UENF



3:30 PM

Characterization of Mortars Incorporated with Natural Acai Fiber: Afonso Azevedo; Marcio Barbosa¹; Higor Azevedo Rocha Rocha²; Markssuel Marvila²; Sergio Monteiro³; ¹Fluminense Federal University; ²Universidade Estadual do Norte Fluminense; ³Military Institute of Engineering

3:50 PM Invited

Renewable Energy for Sustainable Mining: *Tom Xu*¹; Jiann-Yang (Jim) Hwang²; ¹AGreatE Inc; ²Michigan Technological University

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and **Beyond — Superalloys: Mechanical Behavior**

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University



ZTENTS

9



2:00 PM

Damage Mechanisms Involved during Very High Cycle Fatigue of a Coated and Grit-blasted Ni-based Single-crystal Superalloy: Alice Cervellon¹; Luciana Bortoluci Ormastroni²; Tresa Pollock¹; Fernando Pedraza³; Jonathan Cormier²; ¹University Of California Santa Barbara; ²Institut Pprime; ³LaSIE

2:20 PM Invited

Enhancing the Creep Strength of Next Generation Disk Superalloys via Local **Phase Transformation Strengthening**: *Timothy Smith*¹; Timothy Gabb¹; Katelun Wertz²; Joshua Stuckner¹; Laura Evans¹; Ashton Egan³; Michael Mills³; ¹NASA Glenn Research Center; ²AFRL; ³Ohio State University

2:50 PM

Quantifying Deformation Processes Resulting in Local Phase Transformation Strengthening: Ashton Egan¹; Veronika Mazanova¹; Timothy Smith²; Timothy Gabb²; Timothy Hanlon³; Michael Mills¹; ¹Ohio State University; ²NASA Glenn Research Center; ³GE Research

3:10 PM

Solute Segregation at Intrinsic Stacking Faults in Disordered Face-centered Cubic Ni-Co Solid Solution: First-principles and Thermodynamic Modeling: Dongsheng Wen; Longsheng Feng¹; Yunzhi Wang¹; Michael Titus²; ¹The Ohio State University; ²Purdue University

3:30 PM

Partitioning of Cu and Si Contaminants in a Ni-based Superalloy and their Effect on Creep Properties: Martin Detrois¹; Zongrui Pei¹; Kyle Rozman¹; Michael Gao¹; Jonathan Poplawsky²; Paul Jablonski¹; Jeffrey Hawk¹; ¹National Energy Technology Laboratory; ²Oak Ridge National Laboratory

3:50 PM

Deformation of the "'-Ni2(Cr, Mo, W) Phase during Mechanical Testing: Thomas *Mann*¹; Michael Fahrmann²; Michael Titus¹; ¹Purdue University; ²Haynes International

Monday PM March 15, 2021 **MOBILE-FRIEND**

4:10 PM **Mechanical Properties and Microstructural Characterization of Cast Haynes 282** for Advanced Ultra-supercritical (A-USC) Applications: Ling Wang¹; Kinga Unocic¹; Peter Tortorelli¹; Xiang Chen¹; ¹Oak Ridge National Laboratory

4:30 PM

Microstructure and Mechanical Properties of a Centrifugal Cast Ni-Based Alloy: Govindarajan Muralidharan¹; Shivakant Shukla¹; Jim Myers²; ¹Oak Ridge National Laboratory; ²Metaltek International

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Defect Evolution

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory

AB

Π

9

ONTENTS



2:00 PM Invited

Simulation of Intergranular Void Growth under the Combined Effects of Surface Diffusion, Grain Boundary Diffusion, and Bulk Creep: John Sanders¹; Negar Jamshidi¹; Niloofar Jamshidi¹; Mohsen Dadfarnia²; Sankara Subramanian³; James Stubbins⁴; ¹California State University, Fullerton; ²Seattle University; ³PhotoGAUGE; ⁴University of Illinois at Urbana-Champaign

2:30 PM

A Novel Displacement Cascade Driven Irradiation Creep Mechanism in **Pure Copper**: Nargisse Khiara¹; Fabien Onimus¹; Laurent Dupuy¹; Jean-Paul Crocombette¹; Stéphanie Jublot-Leclerc²; Thomas Jourdan¹; Thomas Pardoen³; Jean-Pierre Raskin⁴; Yves Bréchet⁵; ¹CEA Saclay; ²Université Paris–Saclay; ³Ecole Polytechnique de Louvain, Institute of Mechanics, Materials and Civil Engineering (IMMC), Materials and process engineering, Belgium; ⁴Ecole Polytechnique de Louvain; ⁵SIMAP - Science et Ingénierie des MAtériaux et Procédés, Grenoble-**INP**, France

2:50 PM

Controlling Helium Morphology in Pure Metals: Dislocation-helium Interactions: *Calvin Lear*¹; Jonathan Gigax¹; Nan Li¹; Saryu Fensin¹; ¹Los Alamos National Laboratory

3:10 PM

Correlating the Neutron-irradiation Induced Hardening and Solute Nanoclustering in Oxide Dispersion Strengthened Alloys: Samara Levine¹; Arunodaya Bhattacharya²; Andrew Lupini²; David Hoelzer²; Yutai Katoh²; Steven Zinkle¹; ¹Oak Ridge National Laboratory, University of Tennessee; ²Oak Ridge National Laboratory

3:30 PM Invited

Effect of Cr Concentration On <111> and <100> Dislocation Loop Formation in Fe-Cr Alloys: Yaxuan Zhang¹; Ziqi Xiao¹; Xian-Ming Bai¹; ¹Virginia Polytechnic Institute and State University

4:00 PM

Void Swelling and Transmutation in Tungsten Metals and Alloys after Fusion **Relevant Neutron Irradiation**: *Daniel Morrall*¹; John Echols¹; Josina Geringer¹; Lauren Garrison¹; Chad Parish¹; ¹Oak Ridge National Lab

4:20 PM Irradiation Resistance in Several Multi-principal Element Alloys: Yanging Su¹; ¹Utah State University

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ **Experiments and Modeling – Session II**

Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

Monday PM March 15, 2021

Session Chair: Amit Pandey, Lockheed Martin Space



2:00 PM

Low Temperature Failure Mechanism of [001] Niobium Micropillars under **Uniaxial Tension**: Seok-Woo Lee¹; Gyuho Song¹; Nicole Aragon²; Ill Ryu²; ¹University Of Connecticut; ²University of Texas at Dallas

2:20 PM

Quantifying Electron Beam Effects during In-situ TEM Nanomechanical Tensile **Testing on Aluminum Thin Films**: *Sandra Stangebye*¹; Olivier Pierron¹; Joshua Kacher¹; ¹Georgia Institute of Technology

2:40 PM

Deformation Tests of Al Thin Films Using In-situ TEM and Molecular Dynamics Simulations: Lucia Bajtošová¹; Rostislav Králik¹; Barbora Krivská¹; Jozef Veselý¹; Jan Fikar²; Miroslav Cieslar¹; ¹Charles University; ²Ústav Fyziky Materiálu AV CR, v.v.i.

3:00 PM

In-situ TEM Investigation of the Electroplasticity Phenomenon in Ti-6Al: Xiaoqing *Li*¹; Shiteng Zhao²; John Turner²; Karen Bustillo²; Rohan Dhall²; Andrew Minor¹; ¹University of California, Berkeley; ²Lawrence Berkeley National Laboratory

3:20 PM

Giant Superelasticity in SrNi₂P₂ Micropillars via Lattice Collapse and Expansion: Shuyang Xiao¹; Vladislav Borisov²; Guilherme Gorgen-Lesseux³; Gyuho Song¹; Roser Valentí²; Paul Canfield³; Seok-Woo Lee¹; ¹University Of Connecticut; ²Goethe University; ³Iowa State University

3:40 PM

Ripplocations: A Novel Deformation Mechanism in Layered Crystalline Solids: *Hussein Badr*¹; ¹Drexel University



MATERIALS DESIGN

Metal-Matrix Composites: Advances in Analysis, Measurement and **Observations — NanoComposites [Nanoscale + Nanoreinforcements]**

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Srivatsan Tirumalai, The University of Akron; William Harrigan, Gamma Alloys; Simona Hunyadi Murph, Savannah River National Laboratory

Monday PM March 15, 2021

Session Chair: Tirumalai Srivatsan, University of Akron

2:00 PM Keynote A Study Aimed at Understanding the Use of Nanomaterial-treated Filters for the Uptake of Heavy Metals from Water Sources: Simona Hunyadi Murph¹; ¹Savannah **River National Laboratory**

2:40 PM Invited

Strengthening Effects of Multi-walled Carbon Nanotubes and Graphene Nanoplatelets Reinforced in Nickel Matrix Nanocomposites: Amit Patil¹; Tushar Borkar¹; ¹Cleveland State University

3:10 PM Influence of Tungsten Nanopowders on Enhancing the Aging Behavior of a

Copper-chromium Alloy: Gongcheng Yao¹; Shuaihang Pan¹; Xiaochun Li¹; ¹University of California Los Angeles

3:30 PM Invited

In situ Atomic Study of Spontaneous Nanocrystallization of Intermetallic for Interconnection of High-power and Flexible Electronics: *Ying Zhong*¹; Chunging Wang²; Sungho Jin³; ¹University of South Florida; ²Harbin Institute of Technology; ³University of California at San Diego

4:00 PM Invited

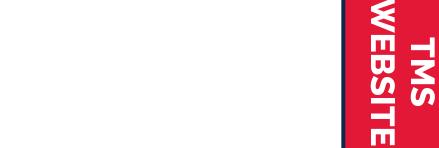
Correlation of Fine Scale Microstructure and Mechanical Properties of Copperalumina Nanocomposites: Ramasis Goswami¹; ¹Naval Research Laboratory

4:30 PM

of Sintering on the Development of Alumina Toughened Influence Nanocomposites: Conventional Versus Microwave: Kunjee Meena¹; Srivatsan *Tirumalai*²; ¹Indian Institute of Technology Roorkee; ²University of Akron

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — **Batteries**



Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

Monday PM March 15, 2021

2:00 PM

BATCircle – Towards CO2 Low Battery Recycling: *Mari Lundstrom*¹; Antti Porvali¹; Heini Elomaa²; Pyry Hannula¹; Pertti Kauranen¹; ¹Aalto University; ²Outotec Reserach Center (Finland) Oy

2:20 PM

Selective Sulfidation and Electrowinning of Nickel and Cobalt for Lithium Ion **Battery Recycling**: Caspar Stinn¹; Antoine Allanore¹; ¹Massachusetts Institute of Technology

2:40 PM

Additive Manufacturing of 3D Microlattice Lithium-ion Battery Electrodes: A **Review**: *Modupeola Dada*¹; Patricia Popoola¹; ¹Tshwane University of Technology

Q



3:00 PM

A Strategy for Acid-free Waste Lithium Battery Processing: Mark Strauss¹; Luis Diaz Aldana¹; Mary Case¹; Tedd Lister¹; ¹Idaho National Laboratory

3:20 PM

The Role of Nickel in Batteries: *Ken Rudisuela*¹: ¹Nickel Institute

3:40 PM

The Effect of Cu, Al and Fe Impurities on Leaching Efficiency of Two Lithium-ion **Battery Waste Fractions**: Alexander Chernyaev¹; *Jere Partinen*¹; Mari Lundström¹; ¹Aalto University

4:00 PM

A Sustainable Oxalate Process for Recovery of Metals from LiCoO₂: Experimental and Modeling Study: Ankit Verma¹; David Corbin¹; Mark Shiflett¹; ¹University of Kansas

4:20 PM

Refining of Mixed Sulphide Precipitate to Produce Battery Grade Metals Using **Outotec Pressure Oxidation Process**: *Christopher Ecott*¹; ¹Outotec

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Martensitic **Transformation**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Monday PM March 15, 2021

Session Chair: Yipeng Gao, Idaho National Laboratory

2:00 PM

Monte Carlo Simulation and Three-dimensional Diffuse Scattering Study of Martensitic Transformation: Xiaoxu Guo¹; Yongmei Jin¹; Yu Wang¹; Yang Ren²; ¹Michigan Technological University; ²Argonne National Laboratory

2:20 PM

Size Effects and Microstructural Evolution of Shape Memory Ceramics during Cyclic Phase Transformations: *Isabel Crystal*¹; Christopher Schuh¹; ¹Massachusetts Institute Of Technology

2:40 PM

Super-critical Elasticity: A Challenge to Martensitic Transformation Theory: Haiyang Chen¹; Yan-Dong Wang¹; Yang Ren²; ¹University of Science and Technology Beijing; ²Argonne National Laboratory

MOBILE-FRIENDL

3:00 PM

Uncovering the Role of Nanoscale Precipitates on Martensitic Transformation and **Superelasticity**: *Shivam Tripathi*¹; Karthik Guda Vishnu¹; Michael Titus¹; Alejandro Strachan¹; ¹Purdue University

MATERIALS PROCESSING

Phonons, Electrons and Dislons: Exploring the Relationships Between Plastic **Deformation and Heat — Session II**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Aashish Rohatgi, Pacific Northwest National Laboratory; Sean Agnew, University of Virginia; Thomas Bieler, Michigan State University

Monday PM March 15, 2021

Session Chairs: Thomas Bieler, Michigan State University; Sean Agnew, University of Viriginia; Aashish Rohatgi, Pacific Northwest National Laboratory

2:00 PM Invited **Do Moving Dislocations Induce Lattice Instabilities?**: Benat Gurrutxaga-Lerma¹; ¹University of Birmingham

2:20 PM Invited Thermal and Strain Rate Effects on Plasticity and Fracture of Gen 3 Steels: Louis Hector¹; ¹General Motors Global Technical Center



MONDAY PM

2:40 PM Invited

Thermo-mechanics of Large Deformation Shear Banding: Curt Bronkhorst¹; Charles Lieou²; Hashem Mourad²; Veronica Anghel²; ¹University of Wisconsin, Madison; ²Los Alamos National Laboratory

3:00 PM

Thermomechanical Conversion in Metals: Dislocation Plasticity Model Evaluation of the Taylor-quinney Coefficient: Charles Lieou¹; Curt Bronkhorst²; ¹Los Alamos National Laboratory; ²University of Wisconsin-Madison

3:20 PM

Unified Analysis of Temperature Fields Arising from Large Strain Deformation and Friction in Manufacturing Processes: Harish Dhami¹; Priti Panda¹; Debapriya Mohanty²; Anirudh Udupa²; James Mann³; *Koushik Viswanathan*¹; Srinivasan Chandrasekar²; ¹Indian Institute of Science; ²Purdue University; ³M4 Sciences Corporation

3:40 PM

Shear Bands, Thermal Profiles and Microstructure Stability in Large-strain **Deformation of High Entropy Alloys**: Shwetabh Yadav¹; Dhruvil Shah¹; Andrew Kustas²; Nicolas Argibay²; Ping Lu²; *Dinakar Sagapuram*¹; ¹Texas A&M University; ²Sandia National Laboratories

NANOSTRUCTURED MATERIALS

Plasmonics in Nanocomposite Materials — From Theory to Application Session



Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Nasrin Hooshmand, Georgia Institute of Technology; Simona Hunyadi Murph, Savannah River National Laboratory; Mahmoud Abdelwahed, The University of Texas at San Antonio

Monday PM March 15, 2021

Session Chair: Sajanlal R Panikkanvalappil, Dana-Farber Cancer Institute

2:00 PM Invited Emerging Anisotropic 2D Layered Materials for Plasmonics and Polaritonics: *Koray Aydin*¹; ¹Northwestern University

2:30 PM Invited Plasmonic Compound Nanohole Arrays: Yiping Zhao¹; ¹University of Georgia

3:00 PM Invited **Electron Transfer and Catalysis in Plasmonic Nanocomposite Systems**: *Patrick Ward*¹; Simona Murph¹; ¹Savannah River National Laboratory

ENERGY & ENVIRONMENT

Powder Materials for Energy Applications – Ceramic Powder Materials



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee

Program Organizers: Kathy Lu, Virginia Polytechnic Institute and State University; Eugene Olevsky, San Diego State University; Hang Yu, Virginia Polytechnic Institute and State University; Ruigang Wang, The University of Alabama; Isabella Van Rooyen, Idaho National Laboratory

Monday PM March 15, 2021

Session Chairs: Eugene Olevsky, San Diego State University; Isabella Van Rooyen, Idaho National Laboratory

2:00 PM

Electric Current Effects in Spark Plasma Sintering: Heating Pathway Analysis: *Eugene Olevsky*¹; Geuntak Lee¹; Charles Maniere¹; Elisa Torresani¹; ¹San Diego State University

2:20 PM

Electrochemical Deposition Synthesis of CeO2 Nanoarrays: *Ruigang Wang*¹; Yifan Wang¹; ¹The University of Alabama

2:40 PM Invited

High Temperature Corrosion and Irradiation Behavior of Silicon Carbide and Nanostructured Ferritic Alloy Composites: *Kaustubh Bawane*¹; Kathy Lu²; Xian-Ming Bai²; Kaijie Ning²; Wei-Ying Chen³; Meimei Li³; ¹Idaho National Laboratory; ²Virginia Tech; ³Argonne National Laboratory

3:10 PM

Oxidation Behaviors of Matrix-grade Graphite in Water Vapor Ingress Accidents for High Temperature Gas-cooled Reactors: Kathy Lu¹; *Yi Je Cho*¹; ¹Virginia Polytechnic Institute and State University

3:30 PM

Simulation of C-SiOC Coatings on Yttria Stabilized Zirconia Microspheres in a Fluidized Bed Coater Based on Multiphase Flow with Interface Exchange: Kathy Lu¹; *Sanjay Kumar*¹; ¹Virginia Polytechnic Institute and State University

MATERIALS DESIGN

Practical Tools for Integration and Analysis in Materials Engineering — Session II

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Titanium Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Adam Pilchak, US Air Force Research Laboratory; Michael Gram, Titanium Metals Corporation; William Joost; Raymundo Arroyave, Texas A&M University; Charles Ward, AFRL/RXM

Monday PM March 15, 2021

2:00 PM Invited

Foundations and Applications of DAMASK: *Philip Eisenlohr*¹; Martin Diehl²; Pratheek Shanthraj³; Franz Roters⁴; Dierk Raabe⁴; ¹Michigan State University; ²KU Leuven; ³The University of Manchester: ⁴Max, Planck Institut für Eisenforschung

³The University of Manchester; ⁴Max-Planck-Institut für Eisenforschung

4:40 PM

2:40 PM

Prisms-plasticity: An Open Source Crystal Plasticity Finite Element Software: *Mohammadreza Yaghoobi*¹; Sriram Ganesan¹; Aaditya Lakshmanan¹; Srihari Sundar¹; Duncan Greeley¹; Shiva Rudraraju²; John E. Allison¹; Veera Sundararaghavan¹; ¹University of Michigan, Ann Arbor; ²University of Michigan; University of Wisconsin-Madison

3:00 PM

A Fast Fourier Transform Based Crystal Plasticity Constitutive Model for Predicting Creep and Rupture Lifetime in Metallic Systems: Nathan Beets¹; Laurent Capolungo¹; Arul Mariyappan¹; Ricardo Lebensohn¹; ¹Los Alamos National Laboratory

3:20 PM

PRISMS-PF: A High Performance Phase-field Modeling Framework to Simulate Microstructure Evolution: *David Montiel*¹; Stephen DeWitt¹; Yanjun Lyu¹; Katsuyo Thornton¹; John Allison¹; ¹University of Michigan

3:40 PM Invited

Tools for Microstructural Analysis Using Computer Vision and Machine Learning: *Elizabeth Holm*¹; Bo Lei¹; Andrew Kitahara¹; Nan Gao¹; Ryan Cohn¹; ¹Carnegie Mellon University

4:20 PM

AMPIS: Automated Materials Particle Instance Segmentation: *Ryan Cohn*¹; Timothy Prost²; Iver Anderson²; Emma White²; Jordan Tiarks²; Elizabeth Holm¹; ¹Carnegie Mellon University; ²Ames Laboratory

MOBILE-FRIEND



A Method to Reconstruct Prior Beta Grain Orientations from Measured Alphaphase Electron Backscatter Diffraction Data: Adam Pilchak¹; ¹US Air Force Research Laboratory

MATERIALS PROCESSING

Rare Metal Extraction & Processing — Li, Co, Au, Ag, PGMs, Te, Na, W, In

Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

Monday PM March 15, 2021

2:00 PM Invited

Environmental Aspects of the Electrochemical Recovery of Tellurium by Electrochemical Deposition-redox Replacement (EDRR): Petteri Halli¹; Marja Rinne¹; Benjamin Wilson¹; Kirsi Yliniemi¹; *Mari Lundstrom*¹; ¹Aalto University

2:20 PM

Sodium Metal from Sulfate: Jed Checketts¹; *Neale Neelameggham*²; ¹Powerball Industries; ²IND LLC

2:40 PM

Preparation of High-grade Ammonium Metatungstate (AMT) as Precursor for

Industrial Tungsten Catalyst: *Alafara Baba*¹; Sadisu Girigisu¹; Mustapha Raji¹; Abdullah Ibrahim¹; Daud Olaoluwa¹; Kuranga Ayinla¹; Christianah Adeyemi¹; Aishat

MOBILE-FRIEND

NTENTS

Π

9

Abdulkareem¹; Abdul Alabi²; Mohammed Abdul³; ¹University of Ilorin; ²Kwara State University, Malete; ³Federal Polytechnic, Offa

3:00 PM Invited Extraction of Platinum Group Metals from Spent Catalyst Material by a Novel Pyro-metallurgical Process: Ana Maria Martinez¹; Kai Tang¹; Camilla Sommerseth¹; Karen Osen¹; ¹SINTEF

3:20 PM

Developed Commercial Processes to Recover Au, Ag, Pt and Pd from E-waste.: *Rekha Panda*¹; Manis Kumar Jha¹; Jae-chun Lee²; Devendra Deo Pathak³; ¹CSIR-National Metallurgical Laboratory; ²Korea Institute of Geosciences and Mineral Resources (KIGAM); ³Indian Institute of Technology (ISM) Dhanbad

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture of Thin **Films**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota: Erica Lilleodden, Helmholtz-Zentrum Geesthacht



TUESDAY AM

Tuesday AM March 16, 2021

Session Chair: Megan Cordill, Erich Schmid Institute

8:30 AM Invited Leveraging Griffith's Energy Balance in Extreme Environments: *Timothy Weihs*¹; ¹Johns Hopkins University

9:10 AM

Fracture-based Reuse of Single Crystal Wafers for High-Efficiency Photovoltaics: *Jie Chen*¹; Corinne Packard¹; ¹Colorado School of Mines

9:30 AM

Modeling Insights into Micro Single-Edge Bend Fracture Toughness Testing of Multilayered Metal-ceramic Cu/TiN and Al/TiN Nanocomposite Thin Films: Daniel Savage¹; Shubhrodev Bhowmik²; Cayla Harvey³; Amit Misra⁴; Nathan Mara⁵; Jeffrey Wheeler⁶; Johann Michler⁷; Siddhartha Pathak⁸; Marko Knezevic²; ¹University of New Hampshire/Los Alamos National Lab; ²University of New Hampshire; ³University of Nevada; ⁴University of Michigan; ⁵University of Minnesota; ⁶ETH Zürich; ⁷Empa, Swiss Federal Laboratories for Materials Science and Technology; ⁸University of Nevada/Iowa State University

9:50 AM Invited

Fracture and Adhesion in Small Scale Devices – Microswitches, Microcantilevers and Micron-thick Films: Maarten De Boer¹; ¹Carnegie Mellon University

10:30 AM

Improving Metal-polymer Adhesion through Alloy Development: Megan Cordill¹; Patrice Krieml¹; ¹Erich Schmid Institute



ADVANCED MATERIALS

10:50 AM Domain Nucleation in Ferroelastic Microcrystals: Competition between Twinning, Slip and Fracture: *Jessica Krogstad*¹; Charles Smith¹; ¹University of Illinois at Urbana-Champaign

ADDITIVE TECHNOLOGIES

2021 Young Innovator in the Materials Science of Additive Manufacturing Award Lecture — 2021 Young Innovator in the Materials Science of Additive Manufacturing Award Lecture

Tuesday AM March 16, 2021

11:00 AM

Introduction of Award Recipient: 2021 Young Innovator in the Materials Science of Additive Manufacturing Award Lecture: *Allison Beese*¹; ¹Pennsylvania State University

11:05 AM Invited Additive Manufacturing of High Temperature Metals: Present and Future Opportunities: *Michael Kirka*¹; ¹Oak Ridge National Laboratory

11:35 AM Question and Answer Period Morderator: Allison Beese, Pennsylvania State University





TUESDAY AM

2D Materials – Preparation, Properties & Applications — Preparation & Properties

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Sufian Abedrabbo, Khalifa University; Amber Shrivastava, Indian Institute of Technology Bombay

Tuesday AM March 16, 2021

Session Chairs: Ramana Chintalapalle, University of Texas - El Paso; Nuggehalli Ravindra (Ravi), New Jersey Institute of Technology

8:30 AM Invited Pressure-induced Formation and Mechanical Properties of 2D Diamond Boron Nitride: *Elisa Riedo*¹; ¹New York University

8:55 AM Keynote Direct Conversion of Carbon into Graphene, Diamond or Q-carbon: A New Frontier in Materials Science and Applications: *Jagdish Narayan*¹; ¹North Carolina State University

9:25 AM

Anisotropic Thermal Conductivity and Associated Heat Transport Mechanism in Roll-to-Roll Graphene Reinforced Copper Matrix Composites: *Kunming Yang*¹; Y.C. Ma¹; Z.Y. Zhang²; J. Zhu²; Yue Liu¹; T.X. Fan¹; ¹Shanghai Jiao Tong University;

TMS



9:45 AM Invited

Controlled Synthesis of Reduced Graphene Oxide-carbon Nanotube Hybrids and Their Applications in The Fabrication of Membranes for Water Purification: Samar Azizighannad¹; Oindrila Gupta¹; *Somenath Mitra*¹; ¹New Jersey Institute of Technology

10:10 AM

Black Phosphorus Ink Formulation for Aerosol Jet Printing of Optoelectronics: *Florent Muramutsa*¹; Samuel Pedersen¹; Joshua Wood²; Chad Husko³; Brian Jaques¹; David Estrada¹; ¹Boise State University; ²Promethean Consulting, LLC; ³Iris Light Technologies

10:30 AM

HighVolumeMechanochemicalSynthesisofBlackPhosphorusforOptoelectronic Applications: Samuel Pedersen¹; Florent Muramutsa¹; Chad Husko²; Joshua Wood³; David Estrada¹; Brian Jaques¹; ¹Boise State University; ²Iris Light Technologies; ³Promethean Consulting

NUCLEAR MATERIALS

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — Challenges and Recent Progresses and in Nuclear Fuels and **Materials Development**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee



TUESDAY AM

ONTENTS

TABLE

9

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Tuesday AM March 16, 2021

Session Chairs: Tyler Gerczak, Oak Ridge National Laboratory; Robert Roach, Idaho National Laboratory

8:30 AM Invited

Materials Selection in Nuclear Applications a Challenge and an Opportunity for Advanced Material Design, Fabrication and Testing: Peter Hosemann¹; Bernd Gludovatz²; Edward Obbard²; Michael Moschetti²; Ashley Reichardt¹; Stuart Maloy³; ¹University of California Berkeley; ²UNSW Sydney; ³Los Alamos National Laboratory

9:00 AM

High power irradiation testing of TRISO MiniFuel-Compacts in HFIR: Tyler *Gerczak*¹; Christian Petrie¹; Jason Harp¹; Grant Helmreich¹; John Hunn¹; Andrew Kercher¹; Zane Wallen¹; Ryan Gallagher¹; Kory Linton¹; Annabelle Le Coq¹; Ryan Latta²; Blaise Collin²; Nicholas Brown³; ¹Oak Ridge National Laboratory; ²Kairos Power; ³University of Tennessee

9:20 AM Invited

Qualification of 316L Stainless Steel Components for ASME Pressure Retaining Applications: David Gandy¹; Marc Albert¹; Stephen Tate¹; Clint Armstrong²; William Cleary²; ¹Electric Power Research Institute; ²Westinghouse Electric Corporation

9:50 AM Invited

Overview of Nuclear Materials Discovery and Qualification Initiative (NMDQi):

TMS

*Robert Roach*¹; ¹Idaho National Laboratory

10:20 AM **Development and Qualification of Ultrafine-grained and Nanocrystalline Steels** for Nuclear Applications: Haiming Wen¹; Andrew Hoffman¹; Maalavan Arivu¹; Rinat Islamgaliev²; ¹Missouri University of Science and Technology; ²Ufa State Aviation **Technical University**

10:40 AM

Development of Assembly Technique for Fuel Specimens for the MARCH-SERTTA TREAT Irradiation Testing Platform: Connor Woolum¹; Lance Hone¹; Korbin Tritthart¹; ¹Idaho National Laboratory

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Titanium

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Tuesday AM March 16, 2021

Session Chair: Nik Hrabe, National Institute of Standards and Technology (NIST)



8:30 AM Invited

Implementing Processing Strategies and Unique Hot Isostatic Pressing Treatments to Control Microstructure, Defect Content, and Mechanical Properties of Electron Beam Melted Ti-6Al-4V: Jake Benzing¹; Nikolas Hrabe¹; Enrico Lucon¹; Timothy Quinn¹; Julius Bonini²; Magnus Ahlfors³; ¹National Institute of Standards and Technology; ²Lucideon M+P; ³Quintus Technologies

9:00 AM

Effect of Oxide and Hydroxide on Cold Spray of Titanium Particles: Mobin Vandadi¹; Arvand Navabi¹; Trevor Bond¹; Nima Rahbar¹; Winston Soboyejo¹; ¹Worcester Polytechnic Institute

9:20 AM

The Inhomogeneous Microstructure and Properties of Ti-6Al-4V Additively Manufactured with Electron Beam Freeform Fabrication: Samuel Present¹; Karen Taminger²; Chris Domack²; Kevin Hemker¹; ¹Johns Hopkins University; ²NASA Langley Research Center

9:40 AM

Quantifying Layer Uniformity in Ti6Al4V Hybrid Additively Manufactured **Samples Using Ultrasound**: *Luz Sotelo*¹; Cody Pratt¹; Rakeshkumar Karunakaran¹; Cody Kanger¹; Michael Sealy¹; Joseph Turner¹; ¹University of Nebraska Lincoln

ADDITIVE TECHNOLOGIES

Additive Manufacturing for Energy Applications III — Additive Manufacturing **Applications in Nuclear**



Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Nuclear Materials Committee

Program Organizers: Isabella Van Rooyen, Idaho National Laboratory; Indrajit Charit, University of Idaho; Subhashish Meher, Idaho National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Kumar Sridharan, University of Wisconsin-Madison; Xiaoyuan Lou, Auburn University

March 16, 2021 **Tuesday AM**

Session Chair: Kumar Sridharan, University of Wisconsin

8:30 AM Invited

Tailored Radiation Responses of 9-12 wt.% Cr Steels Through Additive Manufacturing: *Kevin Field*¹; T.M. Kelsy Green¹; Weicheng Zhong²; Pengyuan Xiu¹; Gabriella Bruno¹; Niyanth Sridharan³; Lizhen Tan²; Maxim Gussev²; Ying Yang²; ¹University of Michigan; ²Oak Ridge National Laboratory; ³Lincoln Electric

8:50 AM

FunctionalAdvancedPrintingsforNuclearIn-pileSensing:KunalMondal¹;Michael McMurtrey¹; ¹Idaho National Laboratory

9:10 AM

Cold Spray Stainless Steel Deposition to Mitigate CISCC in Canisters for Used Nuclear Fuel Storage: Nicholas Pocquette¹; Hwasung Yeom¹; Hemant Agiwal¹; Kenneth Ross²; John Kessler³; Gary Cannell⁴; Frank Pfefferkorn¹; Kumar Sridharan¹; ¹University of Wisconsin Madison; ²Pacific Northwest Research Laboratory; ³J Kessler and Associates LLC; ⁴Fluor Corporation



9:30 AM

A Review of Solution Based Processing Routes for Advanced Nuclear Fuel Materials: *Elizabeth Zell*¹; Milo Gill²; Yazen Alfayez²; Edward Herderick²; Isabella Van Rooyen¹; ¹Idaho National Laboratory; ²The Ohio State University

9:50 AM

Cold Spray Mitigation of Chloride-induced Stress Corrosion Cracking in Austenitic Stainless Steel Welds: Haozheng Qu¹; Timothy Montoya²; Rebecca Schaller²; Eric Schindelholz³; Kyle Johnson⁴; Janelle Wharry¹; ¹Purdue University; ²Sandia National Laboratories; ³The Ohio State University; ⁴VRC Metal Systems

10:10 AM Invited

From Flight to Fission: Additive Manufacturing Advances at GE in Nuclear Energy: Vipul Gupta¹; Andrew Hoffman¹; Xiaoyuan Lou²; Raul Rebak¹; ¹GE Research; ²Auburn University

10:30 AM

Laser Additive Manufacturing of Grade 91 Steel for Affordable Nuclear Reactor **Components with Improved Radiation Tolerance**: *Stuart Maloy*¹; Calvin Lear¹; Osman El-Atwani¹; Peter Hosemann²; Jeff Bickel²; Thomas Lienert³; Tarasankar DebRoy⁴; Tuhin Mukherjee⁴; ¹Los Alamos National Laboratory; ²University of California Berkeley; ³Optomec Inc.; ⁴Penn State University.

10:50 AM

Cold Spray Chromium Deposition for Accident Tolerant Fuel Cladding: Tyler *Dabney*¹; Hwasung Yeom¹; Kyle Quillin¹; Nick Pocquette¹; Yinbin Miao²; Kun Mo²; Laura Jamison²; Kumar Sridharan¹; ¹University of Wisconsin Madison; ²Argonne National Laboratory

11:10 AM

Evaluation of Oxide Dispersion Strengthened (ODS) Steel Fuel Cladding Tubes TMS WEBSITE Manufactured by Cold Spray Technology: *Hwasung Yeom*¹; Vishnu Ramasawmy¹;

Mia Lenling¹; Peter Hosemann²; David Hoelzer³; Stuart Maloy⁴; Kumar Sridharan¹; ¹University of Wisconsin Madison; ²University of California-Berkeley; ³Oak Ridge National Laboratory; ⁴Los Alamos National Laboratory

11:30 AM Densification of Binder Jetted Tungsten through Chemical Vapor Infiltration for Fusion Energy Application: John Echols¹; Amy Elliot¹; Yutai Katoh¹; Lauren Garrison¹; ¹Oak Ridge National Laboratory

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Metals: Applications of Solidification Fundamentals - In Situ Characterization

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Solidification Committee

Program Organizers: Alex Plotkowski, Oak Ridge National Laboratory; Lang Yuan, University of South Carolina; Kevin Chaput, Northrop Grumman; Mohsen Asle Zaeem, Colorado School of Mines; Wenda Tan, University of Utah; Lianyi Chen, University of Wisconsin-Madison

Tuesday AM March 16, 2021

Session Chairs: Mohsen Aisle Zaeem, Colorado School of Mines; Lang Yuan, University of South Carolina



TUESDAY AM

AB

Π

Q

NTENTS

8:30 AM Invited

Characterization of Material Solidification Behaviors in Laser Powder Bed Fusion Using Operando Synchrotron X-ray Imaging: Tao Sun¹; Lianyi Chen²; ¹University of Virginia; ²University of Wisconsin-Madison

9:00 AM

In-situ High-speed X-ray Diffraction Study of Phase Transformation in a Laser-**Processed 420 Stainless Steel**: *Xuan Zhang*¹; Andrew Chihpin Chuang¹; Meimei Li¹; ¹Argonne National Laboratory

9:20 AM

In-situ Observation of Ferritic vs Austenitic Solidification Mode Competition in 316L Laser Powder Bed Fusion Welds with Synchrotron X-ray Diffraction: Joseph Aroh¹; Seunghee Oh¹; Rachel Lim¹; Benjamin Gould²; Andrew Chuang²; P. Chris Pistorius¹; Anthony Rollett¹; ¹Carnegie Mellon University; ²Argonne National Laboratory

9:40 AM

In-situX-rayImagingofMeltFlowDynamicsinLaserMetalAdditiveManufacturing: *Qilin Guo*¹; Cang Zhao²; Minglei Qu¹; Lianghua Xiong³; S. Mohammad H. Hojjatzadeh¹; Luis I. Escano¹; Niranjan D. Parab²; Kamel Fezzaa²; Tao Sun²; Lianyi Chen¹; ¹University of Wisconsin-Madison; ²Argonne National Laboratory; ³Missouri University of Science and Technology

10:00 AM

In Situ Imaging of the Effect of Gas Flowrates on Directed Energy Deposition: Lorna *Sinclair*¹; Yunhui Chen¹; Samuel Clark¹; Oliver Hatt²; Sebastian Marussi¹; Saurabh Shah¹; Robert Atwood³; Martyn Jones⁴; Gavin Baxter⁴; Chu Lun Alex Leung¹; Iain Todd²; Peter Lee¹; ¹University College London; ²University of Sheffield; ³Diamond Light Source Ltd; ⁴Rolls-Royce plc



TUESDAY AM

TABLE

Q

ONTENTS

10:20 AM

Microstructure Evolution and Nanoindentation Measurements after Laser Resolidification of Hypo-eutectic Al-10 at %Cu: Mohammed Alamoudi¹; Vishwanadh Bathula¹; Jörg Wiezorek¹; ¹University of Pittsburgh

10:40 AM

Simultaneous, In-situ Synchrotron X-ray Radiography and Thermal Imaging of Liquid-to-solid Phase Transformation during Laser Fusion Processing of Ti- and **Ni-alloys**: *Rakesh Kamath*¹; Ryan Heldt¹; Logan White¹; David Garcia²; Rongxuan Wang²; Zhenyu Kong²; Kamel Fezzaa³; Tao Sun⁴; Hahn Choo¹; ¹University of Tennessee Knoxville; ²Virginia Polytechnic Institute and State University; ³Argonne National Laboratory; ⁴University of Virginia

11:00 AM

Ultrafast Dynamics of Solidification and Thermal Strain Evolution in Laser Powder Bed Additive Manufacturing Using High Energy X-ray Diffraction: Adrita Dass¹; Chenxi Tian¹; Shonak Bhattacharya¹; Darren Pagan²; Atieh Moridi¹; ¹Cornell University; ²Cornell High Energy Synchrotron Source

11:20 AM

In-situ X-ray Imaging of Porosity Formation in Directed Energy Deposition: Sarah *Wolff*¹; Benjamin Gould²; Aaron Greco²; Tao Sun³; ¹Texas A&M University; ²Argonne National Laboratory; ³University of Virginia

11:40 AM

Undercooling in Laser Powder Bed Fusion Metal Additive Manufacturing: Meelap Coday¹; Minglei Qu¹; Qilin Guo¹; *Lianyi Chen*¹; ¹University of Wisconsin-Madison



ADDITIVE TECHNOLOGIES

Additive Manufacturing: Materials Design and Alloy Development III -- Super Materials and Extreme Environments — Microstructural Aspects

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek **Innovations LLC**

Tuesday AM March 16, 2021

Session Chair: Orlando Rios, University of Tennessee

8:30 AM Invited Microstructure Evolution of Metallic Alloys under Additive Manufacturing **Conditions**: *Amy Clarke*¹; Jonah Klemm-Toole¹; Behnam Aminahmadi¹; Chloe Johnson¹; Alec Saville¹; Brian Rodgers¹; Jeremy Shin¹; Kamel Fezzaa²; Sven Vogel³; Joseph McKeown⁴; Tresa Pollock⁵; Alain Karma⁶; ¹Colorado School of Mines; ²Advanced Photon Source, Argonne National Laboratory; ³Los Alamos National Laboratory; ⁴Lawrence Livermore National Laboratory; ⁵University of California Santa Barbara; ⁶Northeastern University

9:00 AM Invited Solidification Condition and Its Effects on Microstructure in Metal-power Bed Fusion Processes: Yuichiro Koizumi¹; ¹Osaka University



9:30 AM

Exploring the Structure-property Relationships of the Compositionally Graded WxCoCrFeMnNi High-entropy Alloy: *Jonathan Pegues*¹; Michael Melia¹; Benjamin Gould²; Raymond Puckett¹; Shaun Whetten¹; Nicolas Argibay¹; Tomas Babuska¹; Andrew Kustas¹; ¹Sandia National Laboratories; ²Argonne National Laboratory

9:50 AM

Structure-propertyRelationshipsofAdditivelyManufacturedNi-NbBinaryAlloys: *Andrew Kustas*¹; Jonathan Pegues¹; N. Scott Bobbitt¹; Raymond Puckett¹; Morgan Jones¹; Michael Chandross¹; Nicolas Argibay¹; ¹Sandia National Laboratories

10:10 AM

Microstructural and Mechanical Characterization of Additively Manufactured Al-Fe-V-Si: *Paul Wilson*¹; Christopher Meyer¹; Fatmata Barrie¹; ¹The Boeing Company

10:30 AM

Bulk Single Crystals in Cubic Systems Produced via Electron Beam Melting Additive Manufacturing: *Patxi Fernandez-Zelai*¹; Michael Kirka¹; Sebastien Dryepondt¹; Yousub Lee¹; Christopher Ledford¹; ¹Oak Ridge National Laboratory

10:50 AM

A Comparison between In-situ and Ex-situ Mixing of Nanoparticles with a Matrix in Additive Manufacturing of Metal Matrix Composite: *Somayeh Pasebani*¹; Milad Ghayoor¹; Kijoon Lee¹; Yujuan He¹; Chih-hung Chang¹; Brian Paul¹; ¹Oregon State University

MOBILE-FRIEND

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Simulation and Modelling

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

Tuesday AM March 16, 2021

Session Chairs: Andrew Wessman, The University of Arizona; Yousub Lee, Oak Ridge National Laboratory

8:30 AM Invited

Fundamental Investigation of Multi-Principal Element Alloy (MPEA) Design and Processing Research to Explore Additive Manufacturing (AM) Effects: *Iver Anderson*¹; Emma White¹; Duane Johnson¹; Timothy Prost¹; Ralph Napolitano¹; Andrew Kustas²; Nicolas Argibay²; ¹Iowa State University / Ames Laboratory; ²Sandia National Lab-NM

9:00 AM

CALPHAD Based Thermo Kinetic Modeling for Additive Manufacturing (AM): A Case Study for Fusion Based and Supersolidus Liquid Phase Sintering During Binder Jet: Rangasayee Kannan¹; Peeyush Nandwana¹; ¹Oak Ridge National

TMS



MOBILE-FRIEND

9:20 AM

Phase Field Modeling of Powder Densification in Sintering: Rui Dong¹; Wenda *Tan*¹; ¹University of Utah

9:40 AM Invited

Probabilistic Machine Learning Assisted Study of Directed Energy Deposited Alloys: Soumya Nag¹; Yiming Zhang¹; Sreekar Karnati¹; Lee Kerwin²; Eric MacDonald³; Neil Johnson¹; Sathyanarayanan Raghavan¹; Dora Cheung²; Alex Kitt²; Changjie Sun¹; Genghis Khan¹; Chris Williams⁴; Thomas Broderick⁵; Mark Benedict⁵; Brandon Ribic⁶; ¹GE Research; ²EWI - Buffalo Manufacturing Works; ³Youngstown State University; ⁴GE Aviation; ⁵Air Force Research Laboratory; ⁶America Makes

10:10 AM

Prediction of Microstructure and Phase Evolution during Multi-track, Multi-layer **Directed Energy Deposition of H13**: Neil Bailey¹; Christopher Katinas¹; Yung Shin¹; ¹Purdue University

10:30 AM

New Insights on Cellular Structures Strengthening Mechanisms and Thermal Stability of L-PBF Stainless Steel 316L: Thomas Voisin¹; Jean-Baptiste Forien¹; Aurelien Perron¹; Sylvie Aubry¹; Nicolas Bertin¹; Amit Samanta¹; Alexander Baker¹; Y. Morris Wang¹; ¹Lawrence Livermore National Laboratory

10:50 AM

Process Dependent Nanoscale Vanadium Clustering within Martensite Laths in Laser Powder Bed Fused Additively Manufactured Ti6Al4V: Mangesh Pantawane¹; Sriswaroop Dasari¹; Srinivas Mantri¹; Rajarshi Banerjee¹; Narendra Dahotre¹; ¹University of North Texas



TUESDAY AM

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation — Session III**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Tuesday AM March 16, 2021

8:30 AM

CharacterizationandModelingofDeformationTwinninginMgduringCompression and Tension: Zhe Chen¹; Mohammadreza Yaghoobi¹; Veera Sundararaghavan¹; John Allison¹; Samantha Daly²; ¹University of Michigan; ²University of California, Santa Barbara

8:50 AM

Recent Advances in Applying In-situ Electron Microscopy for Local Determination of Crack Processes: Daniel Kiener¹; Markus Alfreider¹; Inas Issa¹; Michael Wurmshuber¹; Michael Burtscher¹; Klemens Schmuck¹; ¹University of Leoben



Advanced High Strength Steels V — Session III

9:10 AM Invited

Materials Science Applications of Four Dimensional-scanning Transmission Electron Microscopy (4D-STEM): Colin Ophus¹; ¹Lawrence Berkeley National Laboratory

9:40 AM

Study of Slip Transmissibility and Its Correlation to Local Geometrically Necessary **Dislocation Content in Grade 1 Pure Titanium**: *Harsha Phukan*¹; Thomas Bieler¹; Ruqing Xu²; Philip Eisenlohr¹; Martin Crimp¹; Carl Boehlert¹; ¹Michigan State University; ²Argonne National Laboratory

10:00 AM

Study of the Effect of Grain Boundary Parameters on the Micro Hall-Petch Slope in Mg Alloys: Mohsen Taheri Andani¹; Aaditya Lakshmanan¹; Veera Sundararaghavan¹; John Allison¹; Amit Misra¹; ¹University of Michigan

10:20 AM

Recent Advances in Bragg Coherent Diffraction for Nanoscale Imaging of Strain: *Ross Harder*¹; ¹Argonne National Laboratory

10:40 AM

Towards Accurate Absolute Stress and Orientation Measurement by Electron Backscatter Diffraction: *Tijmen Vermeij*¹; Johan Hoefnagels¹; ¹Eindhoven University of Technology

ADVANCED MATERIALS

FABLE OF NTENTS



TUESDAY AM

Sponsored by: TMS Structural Materials Division, TMS: Steels Committee

Program Organizers: Ana Luiza Araujo, CBMM North America Inc.; Louis Hector, General Motors Global Technical Center; Igor Vieira, Nucor Steel; Lijia Zhao, ArcelorMittal USA; Krista Limmer, CCDC Army Research Laboratory; Jonah Klemm-Toole, Colorado School of Mines; Sebastien Allain, Institut Jean Lamour; MingXin Huang, University of Hong Kong

Tuesday AM March 16, 2021

8:30 AM

A Spatial Spin Average Approach to Model Austenitic Steels Using First Principle **Calculations**: *Edwin Antillon*¹; Michelle Johannes¹; Noam Bernstein¹; ¹Naval Research Lab

8:50 AM

PhaseEvolutionofTripleNano-precipitateStrengthenedMn-stabilizedAustenitic **Steel**: *Colin Stewart*¹; Richard Fonda²; Keith Knipling²; Patrick Callahan²; ¹National Research Council Associate at the U.S. Naval Research Laboratory; ²U.S. Naval Research Laboratory

9:10 AM

Microstructural Refinement and Homogenization of High Strength Austenitic Steels for Lightweighting Using Equal Channel Angular Pressing: Ibrahim Karaman¹; Matthew Vaughan¹; *Sezer Picak*¹; ¹Texas A&M University

9:30 AM

Role of Metal Carbides in the Formation of Austenite in a High-Ni Martensitic Steel: Chia-Pao Lee¹; Amir Farkoosh¹; Paul Lambert²; David Seidman¹; ¹Northwestern

University; ²Carderock Division, Naval Surface Warfare Center

TUESDAY AM

TABL

Q

NTENTS

9:50 AM

Effects of Cold Rolling on Austenite Formation in a QLT-Treated High-Ni Martensitic Steel: Chia-Pao Lee¹; Amir Farkoosh¹; Paul Lambert²; David Seidman¹; ¹Northwestern University; ²Carderock Division, Naval Surface Warfare Center

10:10 AM Twinning-induced Plasticity of Austenitic Lightweight High-entropy Steel: Hung-Wei Yen¹; Zen-Hao Lai¹; Yi-Hsuan Sun¹; Yi-Ting Lin¹; Jui-Fan Tu²; ¹National Taiwan University; ²China Steel Corporation

ENERGY & ENVIRONMENT

Advanced Magnetic Materials for Energy and Power Conversion Applications - Developments in Magnetic Materials for Sensors and Data Storage

Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

March 16, 2021 **Tuesday AM**

Session Chair: Manh-Huong Phan, University of South Florida



8:30 AM

Engineering of Magnetic Properties and Magnetoimpedance Effect of Fe-rich Microwires by Reversible and Irreversible Stress-annealing Anisotropy: Paula *Corte-Leon*; Valentina Zhukova¹; Juan Maria Blanco²; Mihail Ipatov¹; Arcady Zhukov³; ¹Dept. Phys. Mater., Upv/Ehu; ²Dept. Appl. Phys., Univ. Basque Country; ³Dept. Phys. Mater., Upv/Ehu and Ikerbasque

8:50 AM

Engineering of Magnetic Properties of Co- -rich Microwires by Post-processing : Lorena Gonzalez-Legarreta¹; Valentina Zhukova¹; Mihail Ipatov¹; *Paula Corte-Leon*; Juan Blanco²; Arcady Zhukov³; ¹Dept. Phys. Mater., Upv/Ehu; ²Dept. Appl. Phys., Univ. Basque Country; ³Dept. Phys. Mater., Upv/Ehu and Ikerbasque

9:10 AM

In Pursuit of Antiskyrmions for Energy-Efficient Spintronics: Structural and Magnetic Characterization of Uniaxial [Pt/Co]-based C_{2v} Thin Films: Michael *Kitcher*¹; Marc De Graef²; Vincent Sokalski²; ¹Carnegie Mellon University; ²Carnegie Mellon University

9:30 AM Invited

Kondo-like Behaviour and GMR Effect in Co-Cu Granular Alloys and Multilayers: *Ricardo Lopez Anton*¹; Mihail Ipatov²; Juan Antonio Gonzalez¹; Juan Pedro Andres¹; Julian Gonzalez²; Valentina Zhukova²; Jakub Mino²; Arcady Zhukov²; ¹Universidad de Castilla-La Mancha; ²University of the Basque Country

10:00 AM Invited

Magnetic Real-time Tracking of Coronavirus Progress: A New Approach Utilizing Magnetic Sensor and Machine Learning: Manh-Huong Phan¹; ¹University of South Florida

10:30 AM Invited

Oxide Thin-film Electronics for the Front-end Conditioning of Flexible Magnetic

Field Sensors: Niko Münzenrieder¹; ¹Free University of Bozen-Bolzano



11:00 AM The Development of On-chip-coil Type GSR Sensor: Yoshinobu Honkura¹; Shinpin Honkura¹; *Mizue Uemura*¹; ¹Magnedesign Corp.

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Energy **Conversion with Emphasis on SOFC**

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and **Storage Committee**

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

March 16, 2021 **Tuesday AM**

Session Chairs: Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space

8:30 AM

Experimental and Computational Investigations of the Multiple Impurities Effect on the SOFC Cathode Materials: Rui Wang¹; Hooman Sabarou¹; Yu Zhong¹; ¹Worcester Polytechnic Institute

8:50 AM

Characteristics of Advanced Protective Layer for SOFC Stacks: Jung Pyung Choi¹; John Hardy¹; ¹Pacific Northwest National Laboratory

9:20 AM Invited

Compositionally-stabilized Nickelate-Ceria Composite Oxygen Electrodes for **Reversible Solid Oxide Fuel Cells and Electrolyzers**: *Srikanth Gopalan*¹; Jane Banner¹; Ayesha Aktar¹; ¹Boston University

9:50 AM

Computational Guided Investigations on LSM/YSZ Triple-phase Boundaries: Rui *Wang*¹; Yu Zhong¹; ¹Worcester Polytechnic Institute

10:10 AM

In-situ Cathode Cleaning for Chromium Poisoning Recovery in Solid Oxide Fuel **Cells**: Zhikuan Zhu¹; Michelle Sugimoto¹; Srikanth Gopalan¹; Soumendra Basu¹; Uday Pal¹; ¹Boston University

10:40 AM

Three-dimensional Simulation of Electrochemical Impedance in Solid Oxide Fuel Cell (SOFC) Cathodes and Its Application in Cathode Characterization: Vishwas *Goel*¹; Dalton Cox²; Scott Barnett²; Katsuyo Thornton¹; ¹University of Michigan; ²Northwestern University

CHARACTERIZATION

Advanced Real Time Imaging — Alloys



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

Tuesday AM March 16, 2021

Session Chairs: Wangzhong Mu, KTH Royal Institute of Technology ; Bryan Webler, Carnegie Mellon University

8:30 AM Invited In Situ Thermoelastic Property Evolution of Ni-based Concentrated Solid Solution Alloys under Extremes: Cody Dennett¹; ¹Idaho National Laboratory

8:50 AM

Atomic Scale Processes of Initial Oxidation of Cu and Cu-Ni Alloy Revealed by In Situ Environmental TEM: Meng Li¹; Matthew Curnan¹; Richard Garza¹; Stephen House¹; Wissam Saidi¹; Judith Yang¹; ¹University of Pittsburgh



9:10 AM

In Situ Investigation of the Effect of Ion Irradiation and Carbon Addition in GST on Crystallization and Amorphization Thresholds: Trevor Clark¹; David Adams¹; Khalid Hattar¹; ¹Sandia National Laboratories

9:30 AM

High-velocity Microparticle Impact Modes for Mismatched Metals: *David Veysset*¹; Mostafa Hassani²; Yuchen Sun¹; Keith Nelson¹; Christopher Schuh¹; ¹Massachusetts Institute of Technology; ²Cornell University

9:50 AM

Dynamics of Abnormal Grain Growth in a Particle-containing System Uncovered by Multimodal Three-dimensional X-ray Imaging: *Jiwoong Kang*¹; Ning Lu¹; Nancy Senabulya¹; Nicolas Gueninchault²; Ashwin Shahani¹; ¹University of Michigan; ²Carl Zeiss X-ray Microscopy, Inc.

MATERIALS PROCESSING

Advances in Powder and Ceramic Materials Science — Ceramic Particles and **Powder**



Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Materials Characterization Committee, TMS: Powder Materials Committee

Program Organizers: Bowen Li, Michigan Technological University; Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology; Kathy Lu, Virginia Polytechnic Institute and State University; Rajiv Soman, Eurofins EAG Materials Science LLC; Faqin Dong, Southwest University of Science and Technology; Jinhong Li, China University of Geosciences (Beijing); Ruigang Wang, The University of Alabama; Eugene Olevsky, San Diego State University

March 16, 2021 **Tuesday AM**

Session Chairs: Bowen Li, Michigan Tech; Rajiv Soman, Eurofins EAG Materials Science LLC

8:30 AM Invited Understanding the Role of Electric Field in the Manipulation of Particles in Aqueous Media and Fabrication of Ice-templated Ceramics: Dipankar Ghosh¹; Sashanka Akurati¹; Shizhi Qian¹; Diego Terrones¹; Bharath Gundrati¹; ¹Old Dominion University

8:50 AM Chemical Etch/Modification Effect on CO Oxidation Performance of Ceria Supported Catalysts: Ruigang Wang¹; Yifan Wang¹; ¹The University of Alabama

9:10 AM Layered Ceramic Structures In1+x(Ti1/2Zn1/2)1-xO3(ZnO)m (m = 2, 4, and 6; x =

0.5): Synthesis, Phase Stability and Dielectric Properties: Victor Emmanuel Alvarez *Montano*¹; Subhash Sharma²; Francisco Brown¹; Alejandro Durán³; ¹Universidad De Sonora; ²Catedra CONACYT CNyN-UNAM; ³Universidad Nacional Autonoma de Mexico CNyN-UNAM

9:30 AM

Mineralogical Characteristics of Sepiolite under Thermal Treatment: Huaguang *Wang*¹; Bowen Li¹; ¹Michigan Technological University

9:50 AM

Dielectrophoretic Control of Ceramic Particles for Fabrication of Ice-templated **Structures**: *Bharath Gundrati*¹; Sashanka Akurati¹; Shizhi Qian¹; Dipankar Ghosh¹; ¹Old Dominion University

MATERIALS DESIGN

AI/Data Informatics: Applications and Uncertainty Quantification at Atomistics and Mesoscales — Session III

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Tuesday AM March 16, 2021



10:20 AM

Session Chairs: Mitchell Wood, Sandia national lab; Oliver Johnson, Brigham Young University

8:30 AM

AlGuidedHigh-throughputExplorationofPotentialEnergySurfaces:Subramanian Sankaranarayanan¹; ¹University of Illinois Chicago

9:00 AM

Decision Trees in Continuous Action Space for High-throughput Exploration of Potential Energy Surfaces: Sukriti Manna¹; Troy Loeffler¹; Rohit Batra¹; Suvo Banik¹; Henry Chan¹; Subramanian Sankaranarayanan¹; ¹Argonne National Laboratory

9:20 AM

Building a Better Database to Learn From; Application to Interatomic Potentials: *Mitchell Wood*¹; Nicholas Lubbers²; Danny Perez²; Charles Sievers¹; ¹Sandia National Laboratories; ²Los Alamos National Lab

9:40 AM

Neural Network Reactive Force Field for C, H, N, O Systems: *Pilsun Yoo*¹; Michael Sakano¹; Saaketh Desai¹; Mahbubul Islam²; Peilin Liao¹; Alejandro Strachan¹; ¹Purdue University; ²Wayne State University

10:00 AM

Accelerating Phase-field Predictions via Machine Learning Trained Surrogate Models: David Montes de Oca Zapiain¹; James Stewart¹; *Remi Dingreville*¹; ¹Sandia National Laboratories

ONTENTS

Π

OF



Simultaneous Development and Robust Optimization of a Microstructure Dependent Material Model: Leveraging Sequential Monte-Carlo Methods to Enhance Symbolic Regression Analysis: Karl Garbrecht¹; Nolan Strauss¹; Geoffrey Bomarito²; Patrick Leser²; Jacob Hochhalter¹; ¹University of Utah; ²NASA

10:40 AM

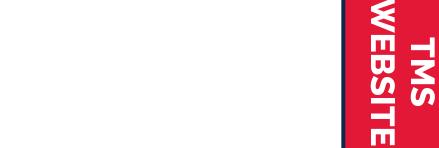
Exploring Metastability and Mapping Metastable Phase Diagrams Using Machine Learning: Srilok Srinivasan¹; Rohit Batra¹; Duan Luo¹; Troy Loeffler¹; Sukriti Manna¹; Henry Chan¹; Liuxiang Yang²; Wenge Yang²; Jianguo Wen¹; Pierre Darancet¹; Subramanian Sankaranarayanan¹; ¹Argonne National Laboratory; ²Center for High Pressure Science and Technology Advanced Research

11:00 AM

Machine Learning Guided Discovery of Novel Oxide Perovskites for Scintillator Applications: Anjana Talapatra¹; Blas Uberuaga¹; Christopher Stanek¹; Ghanshyam Pilania¹; ¹Los Alamos National Laboratory

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering — Large Scale Computational Simulations and Microscale Algorithms for Study Structure-**Processing Relations**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Tuesday AM March 16, 2021

Session Chairs: Cheikh Cisse, Colorado School of Mines; Mohsen Asle Zaeem, Colorado School of Mines

8:30 AM

Exascale-motivated Algorithm Development for Nano and Mesoscale Materials **Methods**: *Samuel Reeve*¹; Matthew Rolchigo¹; Jim Belak¹; ¹Lawrence Livermore National Laboratory

8:50 AM

Preparing for Exascale Phase-field Simulations: Scalable, Performance-portable **Precipitation Simulations**: *Stephen DeWitt*¹; Philip Fackler¹; Younggil Song¹; Bala Radhakrishnan¹; John Turner¹; ¹Oak Ridge National Laboratory

9:10 AM

Tusas: A Modern Computational Approach for Microstructure Evolution Toward **Exascale**: *Supriyo Ghosh*¹; Christopher Newman¹; Marianne Francois¹; ¹Los Alamos



National Laboratory

9:30 AM

Bayesian Data Assimilation for Phase-field Simulation of Solid-state Sintering: *Akimitsu Ishii*¹; Akinori Yamanaka¹; Yuki Okada¹; Akiyasu Yamamoto¹; ¹Tokyo University of Agriculture and Technology

9:50 AM Phase Field Dislocation Dynamics (PFDD) Modeling of Non-Schmid Effects in BCC Metals: Hyojung Kim¹; Nithin Mathew¹; Darby J. Luscher¹; Abigail Hunter¹; ¹Los **Alamos National Laboratory**

10:10 AM

A Quantitative Phase-field Model for Study of Shape Memory Behavior and **Elastocaloric Effect in CuAlBe**: *Cheikh Cissé*¹; Mohsen Asle Zaeem¹; ¹Colorado School of Mines

ELECTRONIC MATERIALS

Alloys and Compounds for Thermoelectric and Solar Cell Applications IX — **Session III**



Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Alloy Phases Committee**

Program Organizers: Hsin-Jay Wu, National Chiao Tung University; Sinn-wen Chen, National Tsing Hua University; Franck Gascoin, Cnrs Crismat Unicaen; Philippe Jund, Montpellier University; Yoshisato Kimura, Tokyo Institute of Technology; Lan Li, Boise State University; Takao Mori, National Institute for Materials Science; Tiejun Zhu, Zhejiang University; Alexandra Zevalkink, Michigan State University; Wan-Ting Chiu, Tokyo Institute of Technology

March 16, 2021 **Tuesday AM**

Session Chairs: Yoshisato Kimura, Tokyo Institute of Technology; Chenguang Fu, **Zhejiang University**

8:30 AM Invited Mg3(Sb,Bi)2 Thermoelectric Single Crystals: From p-type to n-type: Chenguang *Fu*¹; Yu Pan²; Kazuki Imasato³; Mengyu Yao²; Tiejun Zhu¹; G. Jeffrey Snyder³; Claudia Felser²; ¹Zhejiang University; ²Max Planck Institute for Chemical Physics of Solids; ³Northwestern University

8:50 AM Invited

Optimization of n- and p-type Mg2X (X: Si, Ge, Sn): Understanding the Impact of Mg on the Thermoelectric Performance and the Change of the Valence Bands **Under Solid Solution Formation**: *Johannes De Boor*¹; Hasbuna Kamila¹; Mohammad Yasseri¹; Aryan Sankhla¹; Eckhard Müller¹; ¹German Aerospace Center

9:10 AM Invited

PhaseInterfaceFormationInducedbyPhaseSeparationProcessinThermoelectric Mg₂(Si, Sn) Alloys and (Zr, Ti)NiSn Alloys: Yoshisato Kimura¹; Yaw Wang Chai¹; Manabu Watanabe¹; Yonghoon Lee²; ¹Tokyo Institute of Technology; ²KELK Ltd.

9:30 AM

MicrostructureandBandEngineeringfortheHighPerformanceofn-typeMg3Sb2-Mg3Bi2 Alloy: *Kazuki Imasato*¹; G. Jeffrey Snyder¹; ¹Northwestern University

9:50 AM Invited Self-tuning of Carrier Type and Improved Thermoelectric Performance in Skutterudite CoM1.5Te1.5 (M = Sn or Ge): Li-Chyong Chen¹; Suneesh MV²; Ta-Lei Chou²; Kuei-Hsien Chen²; ¹National Taiwan University; ²Academia Sinica

10:10 AM Invited The Doping Effects on the Thermal Conductivity of GeTe: Jie Ma¹; Jiong Yang²; Yangzhong Pei³; Siqi Lin³; ¹Shanghai Jiao Tong University; ²Shanghai University; ³Tongji University

10:30 AM High-performanceGeTe-basedThermoelectricMaterialsviaCarrierOptimization: *Yi-Fen Tsai*¹; Hsin-Jay Wu¹; ¹National Chiao Tung University

10:50 AM

Phase Transition Behavior and Thermoelectric Property of Te doped Cu2Se: Wan-*Ting Yen*¹; Hsin-jay Wu¹; ¹National Chiao Tung University

11:10 AM Invited

FunctionalizationoftheConductiveNetworkandStructuralDisorderEngineering: Two Strategies to Reach High ZT in Ternary and Quaternary Sulfides: Emmanuel *Guilmeau*¹; ¹Laboratoire CRISMAT



11:30 AM

Effect of Structural Disorder on the Thermoelectric Properties of Kesterite (Cu2ZnSnS4): *Eleonora Isotta*¹; Binayak Mukherjee¹; Carlo Fanciulli²; Nicola M. Pugno¹; Paolo Scardi¹; ¹University of Trento; ²CNR-ICMATE, Lecco Unit

LIGHT METALS

Alumina and Bauxite — Novel Processes and Bauxite Residue

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Anne Duncan, Hatch

Tuesday AM March 16, 2021

8:30 AM Invited RevisitingAlternativeSmelterGradeAluminaProductionProcesses:AndreyPanov¹; Alexander Senyuta¹; Andrey Smirnov¹; ¹RUSAL Engineering and Technological Center

9:05 AM Silicon Rich Iron Alloy from Bauxite Residue: *Halvor Dalaker*¹; Casper van der Eijk¹; ¹Sintef

9:25 AM

Bauxite Residue Neutralization Potential Using Biogenic Sulfuric and Citric Acids: Patricia Silva¹; Roseanne Holanda¹; Andre Carmo¹; Fernando Gomes¹; Raphael Costa²; Caio Melo²; *Adriano Lucheta*¹; Marcelo Montini²; ¹SENAI Innovation Institute for Mineral Technologies; ²Norsk Hydro Brasil



9:45 AM

Gravity Methods Applied to Bauxite Residue for Mineral Pre-concentration: Paula Araújo¹; Patricia Silva¹; Andre Carmo¹; Marcus Vinícius Gonçalves²; Raphael Costa³; Caio Melo³; *Adriano Lucheta*¹; Marcelo Montini³; ¹SENAI Innovation Institute for Mineral Technologies; ²SENAI Innvation Institute for Mineral Processing; ³Norsk Hydro Brasil

LIGHT METALS

Aluminum Alloys, Processing and Characterization — Material Processing and Modeling

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Dimitry Sediako, University of British Columbia

Tuesday AM March 16, 2021

Session Chair: Eric Taleff, University of Texas

8:30 AM

Simulations of Wear-induced Microstructural Evolution in Nanocrystalline Aluminum: *Yeqi Shi*¹; Izabela Szlufarska¹; ¹University of Wisconsin-Madison

8:50 AM High-throughput Aluminum Alloy Discovery Using Laser Additive Manufacturing:



University; ²Novelis Global Research and Technology Center

9:10 AM

Manufacturing A206 Aluminum Alloy by Step Sand Casting: Effect of Solidification Time on Mechanical and Surface Properties of the Cast Samples Using Experimental and Simulation Results: Amir Kordijazi¹; Pradeep Rohatgi¹; ¹University of Wisconsin Milwaukee

9:30 AM

Experimental and Numerical Examinations Regarding the Material Flow of **Combined Rolling Extrusion Process**: *Christoph Heinzel*¹; Aleksandr Salnikov²; Sören Müller³; ¹SMS Group GmbH; ²RUSAL; ³FZS - TU Berlin

9:50 AM

Comparison of Simulation and Real Life to Set Up Holistic Approach for Extrusion **Process**: Zeynep Tutku Ozen¹; Mehmet Bugra Güner¹; Osman Halil Çelik¹; Görkem Özçelik¹; Murat Konar¹; Turgay Güler¹; Cem Mehmetalioglu¹; Mustafa Serkan Özcan¹; Tolga Demirkiran¹; ¹ASAS

10:10 AM

ComputationalSimulationofNanoparticleDistributionsinMetalMatrixComposite Casting Processes: Gongyuan Zheng¹; Juergen Jakumeit¹; Thomas Pabel²; Christian Kneissl²; Luca Magagnin³; ¹ACCESS e. V.; ²Austrian Foundry Research Institute (OGI); ³Politecnico di Milano

10:30 AM

Effect of Thermomechanical Processing on Strengthening of the 5181 Alloy (with 0.03 %Sc) Sheets for Preservation of 40 % Improved Strength Compared with **5083**: *Dmitry Fokin*¹; Aleksandr Alabin²; Sergey Valchuk²; Viktor Mann²; Aleksandr Krokhin²; ¹Light Materials and Technologies Institute UC RUSAL; ²JSC RUSAL



MOBILE-FRIENDL

Management

10:50 AM Question and Answer Period

LIGHT METALS

Aluminum Reduction Technology — Cell Operation (Performance and **Operating Advances**)

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Nadia Ahli, Emirates Global Aluminium; Nancy Holt, Hydro Aluminium AS

March 16, 2021 **Tuesday AM**

Session Chairs: Nabeel Al Jallabi, ALBA; Nancy Holt, Hydro Aluminium AS

8:30 AM Carbon Dust - Its Short-Term Influence on Potroom Operations: Matthias Dechent¹; ¹Trimet Aluminium SE

8:50 AM

Experience with Lengthy Pot Hibernation at Alcoa Baie-Comeau: Xiangwen *Wang*¹; Marie-Eve Laframboise¹; Patricia Gagnon¹; Gilles Proulx¹; ¹Alcoa Corp

9:10 AM

Improvement to Alpsys Instability and Alumina Feeding Control: Anne Gosselin¹; ¹Rio Tinto



Session Chairs: Peter Liaw, The University of Tennesee; Jinn Chu, National

9:30 AM

Hydro's New Karmøy Technology Pilot: Start-up and Early Operation: Pierre Reny¹; Martin Segatz¹; Haakon Haakonsen¹; Håvard Gikling¹; Mona Assadian¹; Jan Frode Høines¹; Espen Kvilhaug¹; Asgeir Bardal¹; Erik Solbu¹; ¹Hydro

9:50 AM

AP12 Low Energy Technology at ALRO Smelter: Marian Cilianu¹; Bertrand Allano²; Gheorghe Dobra¹; Ion Mihaescu¹; Claude Ritter²; Andre Auge²; Yves Caratini²; ¹Vimetco alro; ²Rio Tinto

10:10 AM Question and Answer Period

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII — Alloy Development and Application I

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa **Technical Center**

Tuesday AM March 16, 2021

TABLE

Q

NTENTS



MOBILE-FRIENDL

Taiwan University of Science and Technology

8:30 AM Invited **Overview on Additive Manufacturing Techniques for Bulk Metallic Glasses:** *Douglas Hofmann*¹; Punnathat Bordeenithikasem¹; Samad Firdosy¹; Andre Pate¹; Daniel East²; ¹NASA JPL/Caltech; ²CSIRO

8:55 AM

Demisability of Bulk Metallic Glasses for Potential Satellite Applications: *Punnathat Bordeenithikasem*¹; Scott Roberts¹; Douglas Hofmann¹; J. Martin Ratliff¹; Benton Greene²; John Bacon²; Sungwoo Sohn³; Jan Schroers³; ¹NASA Jet Propulsion Laboratory; ²NASA Johnson Space Center; ³Yale University

9:15 AM

Nanomolding Far and Close to Equilibrium: Naijia Liu¹; Guannan Liu¹; Arindam Raj¹; Sungwoo Sohn¹; Jan Schroers¹; ¹Yale University

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Advanced **Characterization Methods II**



Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

Tuesday AM March 16, 2021

Session Chairs: Andrew Brown, Army Research Laboratory; Yunus Kalay, Middle East Technical University

8:30 AM On the Origins of the Discrepancies between Optical, SEM, and EBSD-based Grain Size Measurements: *Eric Payton*¹; Kayla Evans¹; ¹Air Force Research Laboratory

8:50 AM

A Correlative Approach for Distinguishing Multiple BCC Phases in Thick-Section High Strength Steels: *Virgínia Bertolo*¹; Quanxin Jiang¹; Carey Walters²; Jilt Sietsma¹; Vera Popovich¹; ¹Delft University of Technology; ²TNO

9:10 AM

Ultrasonic Scattering in Two-phase Polycrystalline Materials: Showmic Islam¹; Musa Norouzian¹; Joseph Turner¹; ¹University of Nebraska-Lincoln



9:30 AM

Effects of Microstructural Features on the Crack Initiation Mechanism in AA6451 during Three-point Bending: *Yung Suk Yoo*¹; Sazol Das²; Richard Hamerton²; Josh Kacher¹; ¹Georgia Institute of Technology; ²Novelis Inc.

9:50 AM

Applying Stereological Characterisation to the Solidification Structure of Single Crystal Alloys to Deduce the 3D Macroscopic Solid/Liquid Interface Shape: Joel Strickland¹; Bogdan Nenchev¹; Karl Tassenberg¹; Samuel Perry¹; Gareth Sheppard¹; Hongbiao Dong¹; ¹University of Leicester

10:10 AM

Development of Onboard Temperature Monitoring System for Axlebox in Railway Bogie: *Jeongguk Kim*¹; ¹Korea Railroad Research Institute

10:30 AM

Influence of Morphology on Ultrasonic Scattering: A Theoretical Study: Showmic Islam¹; Musa Norouzian¹; Joseph Turner¹; ¹University of Nebraska-Lincoln

10:50 AM

In Situ Study of High Temperature Oxidation of Alloys Using Ambient Pressure X-ray Photoelectron Spectroscopy: *Richard Oleksak*¹; John Baltrus¹; Tao Liu¹; Rafik Addou²; J Trey Diulus²; Gregory Herman²; Bharat Gwalani³; Arun Devaraj³; Ömer Dogan¹; ¹National Energy Technology Laboratory; ²Oregon State University; ³Pacific Northwest National Laboratory

11:10 AM

Characterization of Reactive Metallic Nanolayers through High-speed Imaging: Ali Bagheri Behboud¹; Feyza Kazanc¹; *Sezer Ozerinc*¹; ¹Middle East Technical University



NUCLEAR MATERIALS

Committee



NTENTS

Π

Q

Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University; Joshua Kane, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory; J. Kennedy, Idaho National Laboratory; Arthur Motta, Pennsylvania State University

Characterization of Nuclear Materials and Fuels with Advanced X-ray and

Characterization, Testing, and Simulation Committee, TMS: Nuclear Materials

Program Organizers: Xuan Zhang, Argonne National Laboratory; Jonathan

Neutron Techniques – Neutron Diffraction and Imaging

Sponsored by: TMS Structural Materials Division, TMS: Advanced

Tuesday AM March 16, 2021

Session Chairs: J. Rory Kennedy, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory

8:30 AM Invited

Advanced Characterization of Nuclear Fuel Using Neutron Imaging: Yuxuan Zhang¹; Hassina Bilheux¹; Kristian Myhre¹; Jean Bilheux¹; Jiao Lin²; Jared Johnson¹; Andrew Miskowiec¹; Rodney Hunt¹; Louis Santodonato³; Jamie Molaison¹; Paris Cornwell¹; Erik Stringfellow¹; ¹Oak Ridge National Laboratory; ²Satelytics; ³Advanced Research Systems, Inc.

8:55 AM Invited

NeutronImagingatLANSCE: CharacterizingNuclearMaterialsforNextGeneration Reactor Designs.: *Alexander Long*¹; Sven Vogel¹; ¹Los Alamos National Laboratory

9:20 AM

Characterization of Irradiated Nuclear Fuels with Pulsed Neutrons: *Sven Vogel*¹; Kenneth McClellan¹; Luca Capriotti²; Jason Harp³; Alexander Long¹; Danielle Schaper¹; Eric Larson¹; D. Travis Carver¹; Jay Lin⁴; Peter Hosemann⁴; Thilo Balke⁵; ¹Los Alamos National Laboratory; ²Idaho National Laboratory; ³Oak Ridge National Laboratory; ⁴UC Berkeley; ⁵LANL/Purdue University

9:40 AM

Characterization of the Crystal Structure Evolution of U-Zr Alloys Utilizing Timeof-Flight Neutron Diffraction with In-situ-heating: *Walter Williams*¹; Sven Vogel²; Jianzhong Zhang²; Maria Okuniewski³; ¹Idaho National Laboratory; ²Los Alamos National Laboratory; ³Purdue University

10:00 AM

Microstructure and Crystal Structure Studies in the U-Zr System: *Sven Vogel*¹; Yi Xie²; Luca Capriotti³; Michael Benson³; Jason Harp⁴; ¹Los Alamos National Laboratory; ²Purdue University; ³Idaho National Laboratory; ⁴Oak Ridge National Laboratory

10:20 AM

Non-destructive Characterization of Nuclear Materials using Neutron Imaging Techniques: *Hassina Bilheux*¹; Yuxuan Zhang¹; Jean Bilheux¹; Erik Stringfellow¹; Kristian Myhre¹; Brianne Beers¹; Brent Heuser¹; Tommy Thomasson¹; Amy Jones¹; Richard Ibberson¹; ¹Oak Ridge National Laboratory

10:40 AM

Neutron Radiography Capabilities at LANSCE: Completing LANSCE's Cold/ Thermal/Epithermal Imaging Suite With Fast-neutron Radiography: Danielle



²Nevada National Security Site; ³Sandia National Laboratory

11:00 AM Transmission Spectrum Estimation and Material Decomposition with Energy **Resolved Neutron Imaging**: *Thilo Balke*¹; Alexander Long¹; Sven Vogel¹; Brendt Wohlberg¹; Charles Bouman¹; ¹Los Alamos National Laboratory

NUCLEAR MATERIALS

Composite Materials for Nuclear Applications – Ceramic Composites

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee, TMS: Nuclear Materials Committee

Program Organizers: Anne Campbell, Oak Ridge National Laboratory; Dong Liu, University of Bristol; Rick Ubic, Boise State University; Lauren Garrison, Oak Ridge National Laboratory; Peng Xu, Idaho National Laboratory; Johann (Hans) Riesch, Max Planck Institute for Plasma Physics

March 16, 2021 **Tuesday AM**

Session Chair: Peng Xu, Idaho National Laboratory

8:30 AM Invited

SiGASiC-SiC Composites Development for Accident Tolerant Fuel: Christian Deck¹; Rolf Haefelfinger¹; Jon Sheeder¹; Lucas Borowski¹; Sarah Oswald¹; Joel Kosmatka¹; Ryan Hon¹; Kirill Shapovalov¹; Sean Gonderman¹; Jack Gazza¹; Christina Back¹;



¹General Atomics

9:00 AM

Development of PVD Cr Coatings for Hydrothermal Corrosion Mitigation of SiC-SiC, Fuel Cladding in LWRs: *Kyle Quillin*¹; Hwasung Yeom¹; Tyler Dabney¹; John Lacy¹; Taeho Kim¹; Sergey Chemerisov²; Adrien Couet¹; Kumar Sridharan¹; ¹University of Wisconsin, Madison; ²Argonne National Laboratory

9:20 AM

Corrosion and TEM Analysis of CVD and PVD Coatings for BWR Accident Tolerant Fuel Cladding: *Ryan Schoell*¹; Joey Kabel²; Sebastian Lam³; Kirill Shapovalov⁴; Peter Hosemann³; Djamel Kaoumi¹; ¹North Carolina State University; ²University of California Berkeley ; ³University of California Berkeley; ⁴General Atomics

9:40 AM

Novel Fiber Fretting Technique for Tribological Properties of Composite Interphases: *Joseph Kabel*¹; Thomas Edwards²; Caroline Hain²; Tatiana Kochetkova²; Johann Michler²; Peter Hosemann¹; ¹University of California, Berkeley; ²EMPA

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics – Software Tools and Material Prediction / Thermodynamics and Phase Selection



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

March 16, 2021 **Tuesday AM**

Session Chairs: Prashant Singh, Ames Laboratory; Vahid Attari, Texas A&M University; Enrique Martinez Saez, Clemson University; Carelyn Campbell, National Institute of Standards and Technology

8:30 AM Invited Application of CALPHAD-based Tools for Optimizing AM Microstructures and **Properties**: Carelyn Campbell¹; Mark Stoudt¹; James Zuback¹; Souzan Hammadi²; ¹National Institute of Standards and Technology; ²Royal Institute of Technology (KTH)

9:00 AM

Ga-Sn-Zn Alloys – Thermophysical Properties of Novel Liquid Metals: Alexandra *Dobosz*¹; Tomasz Gancarz¹; ¹Institute of Metallurgy and Materials Science Polish **Academy of Sciences**

9:20 AM Invited

Understanding Phase Stability and Diffusion Kinetics in Structurally Unstable



Phases from First-principles: *Sara Kadkhodaei*¹; ¹University of Illinois at Chicago

9:50 AM

First Principles Thermodynamics of Fe-Cr-Mn Carbides in High-Mn Steels: *Lekshmi Sreekala*¹; Tilmann Hickel¹; Jörg Neugebauer¹; ¹Max-Planck-Institute For Iron Research

10:10 AM

Interplay between Chemical Interactions and Constituent Strain Energy during the Early Stages of Precipitations: Kang Wang¹; Du Cheng¹; Bi-Cheng Zhou¹; ¹University of Virginia

CORROSION

Corrosion in Heavy Liquid Metals for Energy Systems — Materials Compatibility with Liquid Metal Coolants III

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Nuclear Materials Committee

Program Organizers: Osman Anderoglu, University of New Mexico; Alessandro Marino, SCK-CEN; Michael Short, Massachusetts Institute of Technology; Peter Hosemann, University of California; Mike Ickes, Westinghouse Electric Company

Tuesday AM March 16, 2021

Session Chairs: Osman Anderoglu, University of New Mexico; Alessandro Marino, SCK-CEN



Defect and Phase Transformation Pathway Engineering for Desired Microstructures — Invited Presentations

PHYSICAL METALLURGY

Investigation on the Evaporation Rate of Liquid Lead and Radioisotope Retention Capability of Molten Lead as Coolant: Shuprio Ghosh¹; Osman Anderoglu¹; Cemal Cakez¹; Khaled Talaat¹; Keith Woloshun²; Michael Epstein³; Sung Lee⁴; Paolo Ferroni³; Emre Tatli³; Matthew Memmott⁵; ¹University of New Mexico; ²Los Alamos National Laboratory; ³Westinghouse Electric Company, LLC; ⁴Fauske & Associates, LLC; ⁵Brigham Young University

Preliminary Results on the Compatibility of Fe-Cr-Al and Fe-Cr-Al-Mo Steels with Liquid Sodium at 700 °C.

: *Marie Romedenne*¹; Rishi Pillai¹; Bruce Pint¹; ¹ORNL

9:10 AM

9:30 AM

8:50 AM

Electromagnetic Flow Sensor for Heavy Liquid Metals for Energy Systems: Heng *Ban*¹; Osman Anderoglu²; Cetin Unal³; ¹University of Pittsburgh; ²University of New Mexico; ³Los Alamos National Lab

Review of Liquid Metal Corrosion Under Irradiation and Progress Report on the

LBE-Irradiation-Corrosion Experiment (ICE): *Franziska Schmidt*¹; Peter Hosemann¹;

8:30 AM

¹University of California, Berkeley

TUESDAY AM



MOBILE-FRIEND

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Yufeng Zheng, University of Nevada-Reno ; Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Timofey Frolov, Lawrence Livermore National Laboratory; Stoichko Antonov, Max-Planck-Institut für Eisenforschung GmbH; Jessica Krogstad, University of Illinois at Urbana-Champaign; Bin Li, University of Nevada, Reno

March 16, 2021 **Tuesday AM**

Session Chairs: Yufeng Zheng, University of Nevada Reno; Rongpei Shi, Lawrence Livermore National Laboratory

8:30 AM Invited New Insights on Deformation Twinning- Mechanisms and Modeling: Huseyin Sehitoglu¹; ASK Mohammed¹; Orcun Celebi¹; Gorkem Gengor¹; Jessica Krogstad¹; ¹University of Illinois

8:50 AM Invited

Phase Transformation Pathways in High Entropy Alloys or Complex Concentrated Alloys mediated by Defects: Sriswaroop Dasari¹; Bharat Gwalani¹; Yao-Jen Chang²; Deep Choudhuri¹; Stephane Gorsse³; An-Chou Yeh²; Rajarshi Banerjee¹; ¹University of North Texas; ²National Tsing Hua University; ³University of Bordeaux, France

9:10 AM Invited

Microstructure and Tensile Behavior of Nanostructured Gradient TWIP Steel: Jie Ding¹; Zhongxia Shang¹; Jin Li¹; Haiyan Wang¹; *Xinghang Zhang*¹; ¹Purdue University



MOBILE-FRIEND

MATERIALS PROCESSING

Deformation Induced Microstructural Modification – Session III: Computational Studies of Deformation

9:30 AM Invited

Kinetic Monte Carlo Simulations of Solute Clustering in Multicomponent Al Alloys: Mingfei Zhang¹; Zhucong Xi¹; Louis Hector Jr.¹; Chaoming Yang¹; Liang Qi¹; ¹University of Michigan

9:50 AM Invited

Grain Boundary Segregation in Immiscible Alloys: Anisotropy and Trijunction Effects: Anne Barnett¹; Michael Cox¹; Derek Moore¹; Maher Alghalayini¹; Chris Barr²; Khalid Hattar²; Brad Boyce²; *Fadi Abdeljawad*¹; ¹Clemson University; ²Sandia National Laboratories

10:10 AM Invited

Development of Superalloys Driven by Atomic-scale Interactions of Solutes with Crystal Defects: Paraskevas Kontis¹; Stoichko Antonov¹; Philipp Kürnsteiner¹; Shyam Katnagallu²; Jaber Mianroodi¹; Lola Lilensten³; ¹Max-Planck-Institut für Eisenforschung GmbH; ²Karlsruhe Institute of Technology; ³CNRS - Institut de **Recherche de Chimie Paris**

10:30 AM Invited **Evolution of Metastable Grain Boundaries and Its Implications on Nanocrystals'** Hardness Variation: Zhitong Bai¹; Glenn Balbus²; Daniel Gianola²; Yue Fan¹; ¹University of Michigan; ²UCSB



TUESDAY AM

TABLE

9

ONTENTS

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside ; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

March 16, 2021 **Tuesday AM**

Session Chairs: Peter Sushko, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California Riverside

8:30 AM Invited Grain Boundary Segregation in Nanocrystalline Alloys: Multicomponent, Anisotropy, and Stress Effects: Malek Alkayyali¹; Yasir Mahmood¹; Josh Arrington¹; *Fadi Abdeljawad*¹; ¹Clemson University

9:00 AM

Effect of Loading Path on Grain Misorientation Evolution in Polycrystalline Al under Large Deformation: Wenkai Fu¹; Yulan Li¹; Shenyang Hu¹; Peter Sushko¹; Suveen Mathaudhu²; ¹Pacific Northwest National Laboratory; ²Pacific Northwest National Laboratory & University of California, Riverside

9:20 AM

A First Principles Criterion for Microstructure Evolution in Deformation Twinned FCC Materials: Matthew Daly¹; Ritesh Jagatramka¹; Junaid Ahmed¹; ¹University of Illinois at Chicago

9:40 AM Invited

TMS

Microstructure-based Modeling of Impact-Induced Plastic Deformation: Qi

Tang¹; *Mostafa Hassani*¹; ¹Cornell University

TUESDAY AM TABLE OF CONTENTS

10:10 AM Molecular Dynamics Simulations of Defect Structure Evolution under Shear Deformation in Polycrystalline AL: *Nanjun Chen*¹; Shenyang Hu¹; Wahyu Setyawan¹; Peter Sushko¹; Suveen Mathaudhu²; ¹Pacific Northwest National Laboratory; ²University of California, Riverside

10:30 AM

Modeling the Bonding and Structure of Non-metallic Inclusions within a Nickel Matrix during Forging: *Brandon Mackey*¹; Thomas Siegmund¹; Michael Sangid¹; ¹Purdue University

ELECTRONIC MATERIALS

Electronic Packaging and Interconnections 2021 — Solder Joint Intermetallics

Sponsored by: TMS Functional Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Mehran Maalekian, Mat-Tech; Christopher Gourlay, Imperial College London; Babak Arfaei, Ford Motor Company; Praveen Kumar, Indian Institute of Science; Sai Vadlamani, Intel Corporation; Kazuhiro Nogita, University of Queensland; David Yan, San Jose State University

Tuesday AM March 16, 2021

Session Chairs: Kazuhiro Nogita, The University of Queensland; Xin Fu Tan, The University of Queensland



8:30 AM

On Interface Formation in Zr-based BMG /6061 Al Interconnects Joined by µFSSW: David Yan¹; Logan Vahlstrom¹; ¹San Jose State University

8:50 AM

Real-time Observation of the Accelerated Growth of (Cu,Ni)₆**Sn**₅ **on Cu-xNi**: *Xin Tan*¹; Sergey Belyakov²; Te-Cheng Su²; Stuart McDonald¹; Christopher Gourlay²; Hideyuki Yasuda³; Syo Matsumura⁴; Kazuhiro Nogita¹; ¹University of Queensland; ²Imperial College London; ³Kyoto University; ⁴Kyushu University

9:10 AM

Influence of Indium on the Microstructure and Properties of Interfacial IMC in Snrich Solder Joints: Experiments and First Principle Calculations: Amey Luktuke¹; Arun Sundar¹; Nikhilesh Chawla¹; ¹Purdue University

9:30 AM

Atomic Insights into the Role of Dopants in -Cu6Sn5 toward Its Structural Stability: *Wenhui Yang*¹; Xuan Quy Tran¹; Tomokazu Yamamoto¹; Kazuhiro Nogita²; Syo Matsumura¹; ¹Kyushu University; ²University of Queensland

9:50 AM Invited

Reducing Cracking in BGA Solder Joint Cu6Sn5 by Controlling the Reflow Profile: *Kazuhiro Nogita*¹; Flora Somidin²; Keith Sweatman³; Tetsuya Akaiwa³; Tetsuro Nishimura³; Syo Matsumura⁴; Xiaozhou Ye¹; Stuart McDonald¹; ¹University of Queensland; ²Universiti Malaysia Perlis (UniMAP); ³Nihon Superior Co. Ltd.; ⁴Kyushu University

10:10 AM

The Formation and Growth Kinetics of a Peculiar Cu_6Sn_5/Ag_3Sn Composite



²Conquer Electronics

10:30 AM

Reconciling Phase Equilibria and Crystal Structures for the Cu₆Sn₅ Intermetallic in the Cu-Sn System: *Andreas Leineweber*¹; ¹Technical University Bergakademie Freiberg

10:50 AM Interfacial Reaction of Ni-In System and Mechanical Properties of Ni3In7: *Jia-Yi Liao*¹; C. Robert Kao¹; H. T. Hung¹; ¹National Taiwan University

11:10 AM

Microalloying Effects on Intermetallic Compound Growth and Mechanical Reliability of Sn-Bi Solder Joints: *Yaohui Fan*¹; Yifan Wu¹; Travis Dale¹; Sukshitha Achar¹; Hannah Fowler¹; Nilesh Badwe²; Raiyo Aspandiar²; John Blendell¹; Ganesh Subbarayan¹; Carol Handwerker¹; ¹Purdue University; ²Intel Corporation

ENERGY & ENVIRONMENT

Energy Technologies and CO2 Management — Session III

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Energy Committee

Program Organizers: Alafara Baba, University of Ilorin; Lei Zhang, University of Alaska Fairbanks; Donna Guillen, Idaho National Laboratory; Xiaobo Chen, RMIT University; John Howarter, Purdue University; Neale Neelameggham, IND LLC; Cong Wang, Northeastern University; Ziqi Sun, Queensland University



of Technology; Hong Peng, University of Queensland; Yu Lin Zhong, Griffith University

Tuesday AM March 16, 2021

Session Chairs: Hong Peng, University of Queensland; Xiaobo Chen, RMIT University

8:30 AM

Effects on Operational Capabilities and Lifecycle of Commercially Available Liion Batteries Due to Partial Nail Penetration from Drop Hammer Impact Test: *Casey Jones*¹; Bing Li¹; Vikas Tomar¹; ¹Purdue University

8:50 AM

Excitonic Effects in Absorption Spectra of Carbon Dioxide Reduction Photocatalysts: *Tathagata Biswas*¹; Arunima Singh¹; ¹Arizona State University

9:10 AM

Experimental Study and Numerical Modeling of Nanoparticle Injection Technology for Remediating Leaks of CO2 Storage: *Linfei Li*¹; Yige Zhang¹; Mija Hubler¹; Yunping Xi¹; Pania Newell²; ¹University of Colorado Boulder; ²University of Utah

9:30 AM

High Temperature Properties in Ferritic Heat Resistant Steels with Intermetallic Precipitates for High Efficient Heat Recovery Systems: Akio Mitani¹; Mari Miyoseta¹; *Yukio Tachi*¹; ¹Sanyo Special Steel Co., Ltd.

Environmentally Assisted Cracking: Theory and Practice — Hydrogen

Embrittlement

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Tuesday AM March 16, 2021

Session Chairs: Ian Robertson , University of Wisconsin-Madison; Reiner Kirchheim, Georg-August-Universität Göttingen

8:30 AM Invited Hydrogen Embrittlement – A Retrospective Opinion: *Ian Robertson*¹; ¹University of Wisconsin-Madison

9:15 AM

Discrepancy Between Hydrogen-modified Dislocation Structures in the Surface and Interior Grain: *Shuai Wang*¹; Qingqing Sun¹; ¹Southern University of Science and Technology

9:35 AM

Macroscale-based Approaches for Assessing the Influence of Hydrogen on the Deformation Behavior of Polycrystalline Ni: Zachary Harris¹; Sean Agnew¹; James Burns¹; ¹University of Virginia



TUESDAY AM

0

9:55 AM Assessing the Susceptibility of Existing Pipelines to Hydrogen Embrittlement: *Tim Boot*¹; Ton Riemslag¹; Elise Reinton¹; Carey Walters¹; Ping Liu²; Vera Popovich¹; ¹TU Delft; ²INTECSEA BV

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and Computational Modeling — Multi-mechanical Interactions during Extreme Environment Fatigue Loading

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear, University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara

Tuesday AM March 16, 2021

Session Chair: Brian Wisner, Ohio University

8:30 AM

Additively Manufactured Haynes 282 Superalloy Using L-PBF: Heat Treatment

Effect on Mechanical Properties at Room and Elevated Temperatures: Seyed Ghiaasiaan¹; *Nabeel Ahmad*¹; Paul Gradl¹; Samuel Cordner¹; Colton Katsarelis¹;

William Tilson¹; Shuai Shao¹; Nima Shasaei¹; ¹Auburn University

8:50 AM

Quantification of Fatigue Crack Growth Rates and Fatigue-creep Load Interaction Effects of Heterogeneous Fiber Networks via Thresholded Strain Fields: Sarah *Paluskiewicz*¹; Yoon Joo Na¹; Christopher Muhlstein¹; ¹Georgia Institute of Technology

9:10 AM

Rapid Characterization of Cyclic Response of Small-volume Metal Samples Using Spherical Microindentation Stress-strain: Camilla Johnson¹; Soumya Mohan¹; Reji John²; Adam Pilchak²; Surya Kalidindi¹; ¹Georgia Institute of Technology; ²Air Force **Research Laboratory**

9:30 AM

Fatigue Crack Growth in a Ni-rich NiTiHf High Temperature Shape Memory Alloy under Thermomechanical Loading: Behrouz Haghgouyan¹; Benjamin Young¹; Ibrahim Karaman¹; Dimitris Lagoudas¹; ¹Texas A&M University

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Friction Stir Technologies

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St.



Petersburg Polytechnic University

Tuesday AM March 16, 2021

8:30 AM

Effect of Die Geometry on Rate-controlled Friction Extrusion: Xiao Li¹; Md. Reza-E-Rabby¹; Lei Li¹; Ayoub Soulami¹; Glenn Grant¹; Anthony Reynolds²; ¹Pacific Northwest National Laboratory; ²University of South Carolina

8:50 AM

Engineered Metal Matrix Composites Produced Via Co-extrusion for Hightemperature Friction Stir Welding: Paul Brune¹; Greg Hilmas¹; Jeremy Watts¹; ¹Missouri University of Science and Technology

9:10 AM

Residual Stresses and Nanoscale Evolution in AA6061 Produced by Additive Friction Stir-deposition: Luke Brewer¹; Ning Zhu¹; Dustin Avery¹; Paul Allison¹; James Jordon¹; Yan Chen²; Ke An²; ¹University of Alabama; ²Oak Ridge National Laboratory

9:30 AM

Additive Friction Stir Deposition for Repair and Cladding Applications: Hang Yu¹; ¹Virginia Polytechnic Institute and State University

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Eutectic Growth



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

March 16, 2021 **Tuesday AM**

Session Chairs: Nathalie Mangelinck-Noël, Aix Marseille Univ. CNRS, IM2NP UMR 7334; Melis Serefoglu, Koç University; Sabine Bottin-Rousseau, Sorbonne University; Ulrike Hecht, Access e.V.

8:30 AM Invited **Coupled and Decoupled Eutectic Growth in a Transparent Irregular Eutectic** Alloy: Sabine Bottin-Rousseau¹; Samira Mohagheghi²; Silvère Akamatsu¹; Melis Serefoglu²; ¹Sorbonne University; ²Koç University

9:00 AM

Crystal-orientation Maps of Lamellar Eutectic Growth Microstructures in Thin Al-Al2Cu Films Obtained by Laue Microdiffraction: Mehdi Medjkoune¹; Silvère Akamatsu¹; Geoffroy Prévot¹; Jean-Sébastien Micha²; Sabine Bottin-Rousseau¹; ¹Nanoscience institute of Paris; ²European Synchrotron ESRF, CRG IF Beamline **BM32**

9:20 AM

Coexistence of Rod-like and Lamellar Eutectic Growth Patterns: In Situ **Experiments in Microgravity**: *Silvere Akamatsu*¹; Sabine Bottin-Rousseau²; Mathis Plapp³; Victor Witusiewicz⁴; Ulrike Hecht⁴; ¹Cnrs; ²Sorbonne University; ³Ecole Polytechnique; ⁴Access eV

9:40 AM

Phase-field Simulations of the Lamella-to-rod Transition in Eutectic Solidification: *Mathis Plapp*¹; Sabine Bottin-Rousseau²; Silvère Akamatsu²; ¹Ecole Polytechnique, CNRS; ²Sorbonne Université, CNRS

10:00 AM

Orientation Relationships and Pattern Evolution In Directionally Solidified Al-Cu-Mg Ternary Eutectic: Dominic Ezemenaka¹; Amber Genau¹; ¹University of Alabama at Birmingham

10:20 AM Invited Phase Field Modeling of Solidification with Application to Template-directed **Solidification**: Erik Hanson¹; Mojue Zhang¹; Yanjun Lyu¹; David Montiel¹; *Katsuyo Thornton*¹; ¹University of Michigan

10:50 AM

Probing the Growth Dynamics of Eutectic Colonies in Zn-Al via X-ray Video **Microscopy**: Yeqing Wang¹; Jianrong Gao²; *Ashwin Shahani*¹; ¹University of Michigan; ²Northeastern University

11:10 AM

Lamellar Spacing Selection during Oscillatory Eutectic Solidification: Paul Chao¹; Ashwin Shahani¹; ¹University of Michigan

11:30 AM

Phase Field Modeling of Biomineralization?

Microstructure Evolution in Mollusk Shells

VEBSITE TMS

MOBILE-FRIENDL

CONTENTS

TABLE

P

: *Laszlo Granasy*¹; Laszlo Ratkai¹; Tamas Pusztai¹; ¹Wigner Research Centre for Physics

SPECIAL TOPICS

Frontiers of Materials Award Symposium: 2021 Functional Nanomaterials: Translating Innovation into Pioneering Technologies — Session III

Program Organizer: Huanyu Cheng, Pennsylvania State University

Tuesday AM March 16, 2021

8:30 AM Invited Programmable Gold Nanowire Electronic Skins and Tattoos: *Wenlong Cheng*¹; ¹Monash University

9:10 AM Keynote Wearable Gas Sensors with Wireless Communication and RF Energy Harvesting Capabilities: *Huanyu Cheng*¹; ¹Pennsylvania State University

9:50 AM Invited Engineering Self-folding and Shape Morphing in Patterned Materials: David Gracias¹; ¹Johns Hopkins University

10:30 AM Invited Flexible Printable Bioelectronics Devices: Wearable Biosensors and Bioenergy Harvesters: Joseph Wang¹; ¹University California, San Diego



TUESDAY AM

SPECIAL TOPICS

Frontiers of Materials Award Symposium: Low-Dimensional Materials and Interfaces for Next Generation Computing — Session I

Program Organizer: Deep Jariwala, University of Pennsylvania

Tuesday AM March 16, 2021

8:30 AM

Introductory Comments: Frontiers of Materials Award Symposium: Lowdimensional Materials and Interfaces for Next Generation Computing: Deep Jariwala¹; ¹University of Pennsylvania

8:35 AM Invited Gate-tunable Neuromorphic Devices Enabled by Low-dimensional Materials: Mark Hersam¹; ¹Northwestern University

9:15 AM Keynote 2D/3D Heterostructures for Low-power Logic and Memory Devices: Deep Jariwala¹; ¹University of Pennsylvania

9:55 AM Invited Ferroelectrics: From Memory to Computing: *Suman Datta*¹; ¹University of Notre Dame

Greater Than the Sum of Its Parts — Concurrent Alloy Design and Processing



Science: An LMD Symposium Honoring Raymond Decker — Session II

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Eric Nyberg, Tungsten Heavy Powder & Parts; J. Brian Jordon, University of Alabama; Wilhelmus Sillekens, European Space Agency; Neale Neelameggham, IND LLC; Vineet Joshi, Pacific Northwest National Laboratory

March 16, 2021 **Tuesday AM**

Session Chair: Victoria Miller, University of Florida

8:30 AM Invited **Thixomolded Magnesium: Quick, Light, and Mighty**: *Tracy Berman*¹; ¹University of Michigan

9:00 AM Invited Magnesium Sheet Alloy Development for Room Temperature Forming: Alan Luo¹; Renhai Shi¹; Jiashi Miao¹; Thomas Avey¹; ¹Ohio State University

9:30 AM

Impacts of Grain Boundary Particle Characteristics on Twin Transmission: *Benjamin Anthony*¹; Brandon Leu²; Irene Beyerlein²; Victoria Miller¹; ¹University Of Florida; ²University of California Santa Barbara

9:50 AM Keynote Evolution of Alloy Design, It's Science/Instruments Base, Tech Transfer Routes

and Market Pull, 1921-2021: Raymond Decker¹; ¹University of Michigan

10:35 AM Break

10:55 AM Panel Discussion

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Heterostructured Materials III: Processing and **Properties**

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

Tuesday AM March 16, 2021

Session Chairs: Andrea Hodge, University of Southern California; Megumi Kawasaki, Oregon State University; Nobuhiro Tsuji, Kyoto University

8:30 AM Invited Heterogenous Nanostructured Nickel Superalloy: Andrea Hodge¹; ¹University of Southern California

TMS

ADVANCED MATERIALS

Mechanical Properties I

10:25 AM **Optimizing Wear and Corrosion Resistance of Metallic Multilayers through** Atomic-scale Design: Wenbo Wang¹; Wenjun Cai¹; ¹Virginia Polytechnic Institute and State University

10:00 AM Invited Solid-tsate Additive Manufacturing of Heterostructured Materials via Additive **Friction Stir Deposition**: Hang Yu¹; ¹Virginia Polytechnic Institute and State University

9:35 AM Invited

¹Kyoto University

Metastable Aluminum-magnesium: Megumi Kawasaki¹; ¹Oregon State University

Nucleation of New Deformation Modes in Nanostructured Metals: Nobuhiro Tsuji¹;

9:15 AM Mechanical Properties and Structural Stability of a Bulk Nanostructured

Interface Affected Plasticity in Accumulative Roll Bonded FCC/BCC Metallic Laminates: Rodney McCabe¹; Matthew Schneider¹; Jonathan Gigax¹; Nan Li¹; Thomas Nizolek¹; John Carpenter¹; ¹Los Alamos National Laboratory

CONTENTS

TABLE

9

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

High Entropy Alloys IX: Alloy Development and Properties — Structures and

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Tuesday AM March 16, 2021

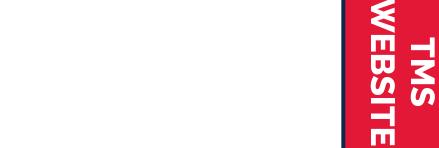
Session Chairs: Lei Lu, Institute of Metal Research, Chinese Academy of Sciences; Hyoung Kim, Pohang University of Science and Technology

8:30 AM Keynote Current Perspectives in High Entropy Alloys: Diran Apelian¹; Benjamin Macdonald¹; Cheng Zhang¹; Enrique Lavernia¹; ¹University of California, Irvine

9:00 AM Invited FCC-HCP Transformation in Cr-Mn-Fe-Co-Ni High Entropy Alloys:- Mechanical **Property and Nanograin Formation**: *Koichi Tsuchiya*¹; Jangho Yi¹; Baozhen Jiang¹; Je In Lee²; ¹National Institute for Materials Science; ²Pusan National University

9:25 AM

Low Cycle Fatigue Behavior and Cyclic Plastic Response of Equiatomic CrCoNi Medium-entropy Alloy: *Milan Heczko*¹; Veronika Mazanova¹; Connor Slone¹; Ivo Kubena²; Jiri Tobias²; Tomas Kruml²; Easo George³; Maryam Ghazisaeidi¹; Jaroslav Polak²; Michael Mills¹; ¹The Ohio State University; ²Institute of Physics of Materials CAS; ³Oak Ridge National Laboratory



MOBILE-FRIENDL

I ENIS

Π

9

9:45 AM Invited Deformation Twinning in FCC High- and Medium-entropy Alloys: *Haruyuki Inui*¹; Koudai Niitsu¹; Kyosuke Kishida¹; ¹Kyoto University

10:10 AM Invited High-strain-rate 2000% Superplasticity in A

nanostructured High-entropy Alloy: *Hyoung Seop Kim*¹; Nhung Thi-Cam Nguyen¹; Peyman Asghari-Rad¹; Praveen Sathiyamoorthi¹; Alireza Zargaran¹; Chong Soo Lee¹; ¹Pohang University of Science and Technology

10:35 AM

IntermediateTemperaturePrecipitationintheHfNbTaTiZrMulti-principalElement Alloy: Megan Emigh¹; Noah Phillips²; Leah Mills²; Sean Murray²; Tresa Pollock¹; ¹University of California, Santa Barbara; ²ATI Specialty Alloys and Components

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling — Structures and Modeling III

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center



TUESDAY AM

Tuesday AM March 16, 2021

Session Chairs: Michael Gao, National Energy Technology Lab; Louis Santodonato, Advanced Research Systems

8:30 AM Invited

Phase Stability of High Entropy Alloys: Effects of Pressure and Temperature: *Michael Gao*¹; Xuesong Fan²; Sita Ram Aryal³; Lizhi Ouyang³; Peter Liaw²; Jeffrey Hawk¹; David Alman¹; ¹National Energy Technology Laboratory; ²University of Tennessee; ³Tennessee State University

8:55 AM Invited Monte Carlo Study of the Entropy Hypothesis Associated with High-entropy Alloys: Louis Santodonato¹; *Peter Liaw*²; ¹Advanced Research Systems; ²University of Tennessee

9:20 AM Invited Core Effect of Local Atomic Configuration and Design Principles in AlxCoCrFeNi High-entropy Alloys: Yu-Chia Yang¹; *Zhenhai Xia*¹; ¹University of North Texas

9:45 AM

Atomistic Modeling of Screw Dislocations in Body-centered Cubic High-entropy Alloys: Sheng Yin¹; Jun Ding¹; Mark Asta¹; Robert Ritchie¹; ¹Lawrence Berkeley National Laboratory

10:05 AM

Can We Control Lattice Distortions in Entropy-stabilized Oxides?: *Keivan Esfarjani*¹; Jonathan Kaufman¹; ¹University of Virginia

TMS /EBSITI

MATERIALS PROCESSING

High Temperature Electrochemistry IV — Session II

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Guy Fredrickson, Idaho National Laboratory

March 16, 2021 **Tuesday AM**

Session Chair: Vasant Kumar Ramachandran, University of Cambridge

8:30 AM

Electrochemical Reactions of Oxide Ions with Tungsten in Molten CaCl.: Chao Zhang¹; Devin Rappleye¹; *Michael Simpson*²; ¹Lawrence Livermore National Laboratory; ²University of Utah

9:00 AM

Optimizing Reaction Selectivity in High Temperature Molten Electrolytes: *Mary Elizabeth Wagner*¹; Antoine Allanore¹; ¹Massachusetts Institute of Technology

9:30 AM

Fundamental Challenges for the Development of Electrolytic Reduction of Uranium Oxide in Molten LiCl-Li2O: Jarom Chamberlain¹; Adam Burak¹; Mario Gonzalez¹; Michael Simpson¹; ¹University of Utah

10:00 AM

MOBILE-FRIEND

New Electrochemical Deoxidation Method of Ti Metal in Molten Salts Containing YCL₃: Akihiro lizuka¹; Takanari Ouchi¹; Toru Okabe¹; ¹The University of Tokyo

MATERIALS DESIGN

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session III

Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

March 16, 2021 **Tuesday AM**

Session Chair: Wei Zhong, University of Maryland

8:30 AM Invited **Unexpected Phenomena Observed in Metallurgical Studies**: Sinn-wen Chen¹; ¹National Tsing Hua University

9:10 AM Invited High-throughput Hot-isostatic-pressing Micro-synthesis for Accelerated Studies of High Entropy Alloys: Lei Zhao¹; Shuying Chen²; Zi Wang³; Lixia Yang¹; Hui Wang¹; Haizhou Wang¹; *Liang Jiang*²; ¹Central Iron & Steel Research Institute, China; ²Yantai University; ³Central South University

9:50 AM Invited

Integration of Computational Tools and Advanced Characterization Methods

TMS WEBSITE

to Understand Phase Transformations in Additively Manufactured Steels: Greta

Tuesday AM March 16, 2021

Lindwall¹; Niklas Holländer Pettersson¹; Chia-Ying Chou¹; Durga Ananthanarayanan¹; Benjamin Neding¹; Peter Hedström¹; Fan Zhang²; ¹KTH Royal Institute of Technology; ²NIST

10:30 AM Invited **Computational Thermodynamics and Its Applications**: *Zi-Kui Liu*¹; ¹Pennsylvania State University

11:10 AM Invited High-throughput Experiments and Machine Learning Modeling for Designing **Next Generation Superalloys**: *Akane Suzuki*¹; Chen Shen¹; ¹GE Research

NUCLEAR MATERIALS

Materials and Chemistry for Molten Salt Systems — Loops and Irradiation **Effects**

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short, Massachusetts Institute of Technology; Raluca Scarlat, University of California-Berkeley





8:30 AM

Corrosion and Mass Transfer of 316H Stainless Steel in Flowing FliNaK Salt: Stephen Raiman¹; Matthew Kurley²; Dino Sulejmanovic²; Scott Nelson²; James Keiser²; Bruce Pint²; ¹Texas A&M University; ²Oak Ridge National Laboratory

8:50 AM

Dutch Molten Salt Irradiation Program: *Ralph Hania*¹; Uazir Bezerra de Oliveira¹; ¹NRG

9:10 AM

Design of Molten Salt Static Corrosion Experiments to Predict Phenomena Relevant to Corrosion in Non-isothermal Nuclear Reactor Salt Loops: Raluca *Scarlat*¹; ¹University of California, Berkeley

9:30 AM

Structural Health Impacts Due to Exposure of Irradiated Molten Chloride Salts: Nora Dianne Ezell¹; *Stephen Raiman*²; Joel McDuffee¹; Matt¹; ¹Oak Ridge National Laboratory; ²ORNL

9:50 AM

Alloy Compatibility in Flowing Cl and F Salts: Bruce Pint¹; Dino Sulejmanovic¹; J. Kurley¹; Stephen Raiman¹; ¹Oak Ridge National Laboratory

10:10 AM

Chemical Effects of Ionizing Radiation on Molten Salt Systems: Simon Pimblott¹; Ruchi Gakhar¹; Gregory Horne¹; Kazihiro Iwamatsu²; Alejandro Ramos³; Jay LaVerne³; James Wishart²; ¹Idaho National Laboratory; ²Brookhaven National Laboratory; ³University of Notre Dame



NTENTS Π

Q

10:40 AM

Microstructural Characterization of Grain Boundaries in Hastelloy N Corroded in Molten FLiBe Salt under Neutron Irradiation: Guiqiu Zheng¹; David Carpenter¹; ¹Massachusetts Institute of Technology

11:00 AM

Exploration of the Corrosion Morphologies of Ni-Cr Alloys in Molten Fluoride Salts with/without Radiation: Weiyue Zhou¹; Yang Yang²; Miaomiao Jin³; Andrew Minor²; Michael Short¹; ¹Massachusetts Institute of Technology; ²Lawrence Berkeley National Laboratory; ³Idaho National Laboratory

11:20 AM

Release Behavior of Tritium Generated inside FLiNaBe by Thermal Neutron: *Kazunari Katayama*¹; ¹Kyushu University

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Polymer Materials and Processes

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao, University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology



Company Ltd.; Shadia Ikhmayies

March 16, 2021 **Tuesday AM**

Session Chairs: Sergio Monteiro, Military Institute of Engineering; Gele Qing, Shougang Group

8:30 AM Keynote Improved Ballistic Armor with Composites Reinforced with Natural Fibers **Functionalized with Graphene Oxide**: Sergio Monteiro¹; Fernanda da Luz¹; Fabio Garcia Filho¹; ¹Military Institute of Engineering

8:50 AM Invited

Tensile Properties of Epoxy Matrix Reinforced with Fique Fabric: Michelle Oliveira; Fabio Garcia Filho¹; Fernanda da Luz¹; Artur Pereira¹; Luana Cristyne Demosthenes¹; Lucio Fabio Nascimento¹; Sergio Monteiro¹; ¹Military Institute of Engineering

9:10 AM Invited

Blending of Polystyrene-block-poly(ethylene-ran-butylene)-block-polystyrene with Polyethylene-graft-polystyrene for Cation Exchange Membrane Preparation with Enhanced Properties: Zhichao Chen¹; Jiann-Yang Hwang²; Yong Shi³; Di Huang²; Weigang Zhao³; ¹Futianbao Environmental Protection Technology Ltd; ²Michigan Technological University; ³Futianbao Environmental protection technology

9:30 AM

Novel Route of Polymerization for Engineering Thermorrigid Biopolymer Based on Soybean Oil

: João Gabriel Rodrigues¹; Karollyne Monsores¹; Suzane Oliveira¹; *Sergio Monteiro*¹; Ricardo Weber¹; ¹Military Institute of Engineering



9:50 AM

Novel Ballistic Composites: Performance Evaluation of Epoxy Composite Reinforced with Buriti Fabric as Component of a Multilayer Armor System: Luana *Cristyne Demosthenes*¹; Lucio Fabio Nascimento¹; Michelle Oliveira¹; Fabio Garcia Filho¹; Fernanda da Luz¹; Ulisses Costa¹; Sergio Monteiro¹; Artur Pereira¹; Fabio Braga²; ¹Military Institute of Engineering; ²Fluminense Federal University

10:10 AM

Barcol Hardness of Green Composites for Cold Repair in Industrial Piping: Felipe Lopes¹; Noan Tonini Simonassi¹; Carlos Fontes Vieira¹; Sergio Neves Monteiro¹; ¹Universidade Estadual do Norte Fluminense

10:30 AM Invited

Comparison of Mechanical Properties of Banana Fibers Reinforcement in **Different Thermoset Matrix Composites**: *Fabio Garcia Filho*; Michelle Oliveira¹; Foluke de Assis¹; Artur Pereira¹; Fernanda da Luz¹; Luana Cristyne Demosthenes¹; Sergio Monteiro¹; ¹Military Institute of Engineering

10:50 AM

Tensile Strength of Synthetic and Green Composites Used as Wrapping Cold **Repair in Piping**: *Felipe Lopes*¹; Noan Tonini Simonassi¹; Carlos Fontes Vieira¹; Sergio Neves Monteiro¹; ¹Universidade Estadual do Norte Fluminense

11:10 AM

Influence of Mercerization Process on the Surface of Coconut Fiber for Composite **Reinforcement**: Géssica Nicolau¹; Ricardo Weber¹; Sergio Monteiro¹; Gabriela Loureiro¹; Amanda Lavinsky¹; Letícia da Fonseca¹; Eduardo da Silva¹; Pedro Luiz dos Santos¹; Rodrigo Abranches¹; Vinícius Machado¹; ¹Military Institute of Engineering



MOBILE-FRIENDL

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and **Beyond — Superalloys: Beyond Nickel-based Superalloys**

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Tuesday AM March 16, 2021

8:30 AM Invited

Accelerated Design of '-strengthened Co-base Superalloys with Improved **Comprehensive Performances**: *Qiang Feng*¹; Longfei Li¹; Wendao Li¹; Min Zou¹; Xiaoli Zhuang¹; Ji-Cheng Zhao²; ¹University of Science & Technology Beijing (USTB); ²University of Maryland

9:00 AM

Effects of Key Elements Ni, Cr and W on High-temperature Microstructural Stability of Multicomponent Co-base Superalloys: Longfei Li¹; Wendao Li¹; Min Zou¹; Qiang Feng¹; Ji-Cheng Zhao²; ¹University of Science & Technology Beijing (USTB); ²University of Maryland



MOBILE-FRIEND

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Process Technology and Modeling Committee

Materials Processing Fundamentals — Molten Metal Processing and Modeling

MATERIALS PROCESSING

11:10 AM **Direct Production of Complex Metallic Alloys**: Jawad Haidar¹; ¹Kinaltek Pty Ltd.

10:50 AM Inverse Design of Chemistry of High Temperature Ni-base Superalloys Using **CALPHAD and Machine Learning**: *Rajesh Jha*; George Dulikravich¹; ¹Florida International University

10:30 AM

Modeling Planar Fault Energies in Ordered D022 Structures: K V Vamsi¹; Tresa Pollock¹; ¹University of California Santa Barbara

Potential: *Tresa Pollock*¹; ¹University of California, Santa Barbara

9:20 AM Invited

Experimentally Determined Creep Properties of Various Alloys and Conclusions for Beyond Nickel-based Superalloys: Uwe Glatzel¹; ¹University Bayreuth

9:50 AM Keynote

Metallic Materials Beyond Nickel-base Superalloys: The Challenges and **TUESDAY AM**





Program Organizers: Jonghyun Lee, Iowa State University; Samuel Wagstaff, Oculatus; Alexandra Anderson, Gopher Resource; Fiseha Tesfaye, Abo Akademi University; Guillaume Lambotte, Boston Metal; Antoine Allanore, Massachusetts Institute of Technology

Tuesday AM March 16, 2021

Session Chair: Jonghyun Lee, Iowa State University

8:30 AM

Contactless Inductive Flow Tomography for Control of Liquid Metal Flow with **Electromagnetic Actuators**: *Ivan Glavinic*¹; Matthias Ratajczak¹; Frank Stefani¹; Sven Eckert¹; Thomas Wondrak¹; ¹Helmholtz-Zentrum Dresden-Rossendorf

8:50 AM

X-ray and Neutron Radiographic Experiments on Particle-laden Molten Metal Flows: Tobias Lappan¹; Martinš Sarma¹; Sascha Heitkam²; David Mannes³; Pavel Trtik³; Natalia Shevchenko¹; Kerstin Eckert²; Sven Eckert¹; ¹Helmholtz-Zentrum Dresden-Rossendorf; ²Technische Universität Dresden; ³Paul Scherrer Institut

9:10 AM

Computational Fluid Dynamics Modeling of Damped Oscillations of Molten Metal **Droplets**: *Ali Rabeh*¹; Makrand Khanwale¹; Baskar Ganapathysubramian¹; Michael SanSoucie²; Jonghyun Lee¹; ¹Iowa State University; ²NASA MSFC

9:30 AM

Numerical Simulation of the Influence of Particle Physical Properties on Flow Field during the Aeration Leaching Process: Mingzhao Zheng¹; Qiuyue Zhao¹; Zimu Zhang¹; Lei Zhou¹; Tingan Zhang¹; ¹Northeastern University

EBSITE

TMS





Mechanical Behavior of Nuclear Reactor Components — Small Scale Testing

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory

March 16, 2021 **Tuesday AM**

8:30 AM Invited In-situ Micro-tensile Studies on the Effects of Ion Irradiation on the Mechanical **Properties of Small-grained Alloys**: *Dhriti Bhattacharyya*¹; Alan Xu¹; Mihail Ionescu¹; Tao Wei¹; Michael Saleh¹; ¹Australian Nuclear Science and Technology Organization

9:00 AM

Bridging the Length Scales via Femtosecond Laser Machining of Micromesoscale Tensile Specimens: Andrew Dong¹; Hi Vo¹; Peter Hosemann¹; Stuart Maloy²; ¹University of California, Berkeley; ²Los Alamos National Laboratory

9:20 AM

a' Precipitation and Hardness Change in Ion Irradiated High Purity FeCr Alloys: *Yajie Zhao*¹; Arunodaya Bhattacharya²; Cristelle Pareige³; Pengcheng Zhu¹; Caleb Massey²; Philip Edmondson²; Jean Henry⁴; Steven Zinkle¹; ¹The University of Tennessee; ²Oak Ridge National Laboratory; ³GPM, Université et INSA de Rouen; ⁴CEA, DEN, Service de Recherches Métallurgiques Appliquées, Laboratoire d'Analyse Microstructurale des Matériaux, Université Paris-Saclay

9:40 AM Invited

Nanomechanical Assessment of a Neutron Irradiated U-10Zr Fuel: Maria Okuniewski¹; Jonova Thomas¹; Alejandro Figueroa¹; Fei Tang²; Daniel Murray²; Xiang Liu²; ¹Purdue University; ²Idaho National Laboratory

10:10 AM

Challenges to Accurate Evaluation of Bulk Hardness with Nanoindentation **Testing at Low Indent Depths**: *Pengcheng Zhu*¹; Yajie Zhao¹; Shradha Agarwal¹; Steven Zinkle¹; ¹University of Tennessee

10:30 AM

High Throughput Assessment of Creep Behavior of Advanced Alloys for Model **Development and Validation**: *Moujhuri Sau*¹; Zezhou Li¹; Eric Hintsala²; Douglas Stauffer²; Laurent Capolungo³; Nathan Mara¹; ¹University of Minnesota; ²Bruker Corporation; ³Los Alamos National Labs

10:50 AM

Creep Behavior of Helium Implanted Submicron Films under Irradiation: Nargisse *Khiara*¹; Michaël Coulombier²; Fabien Onimus¹; Jean-Pierre Raskin²; Thomas Pardoen²; Yves Bréchet³; ¹CEA Saclay; ²Ecole Polytechnique de Louvain; ³Science et Ingénierie des MAtériaux et Procédés

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ Experiments and Modeling — Session III

TMS



Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

March 16, 2021 **Tuesday AM**

Session Chair: Minh-Son Pham, Imperial College

8:30 AM Keynote Observation of Microstructure Evolution in Pure Copper and Copper-8 wt. % Aluminium Alloy during Deformation: Sandhya Verma¹; Prita Pant¹; M P Gururajan¹; ¹Indian Institute of Technology Bombay

9:10 AM

Sub-surface Microtensile Testing in Oxidized Equiatomic Alloy NbTiCr: Robert Wheeler¹; Todd Butler²; Marc Doran³; Scott Apt³; Melinda Ostendorf³; ¹Microtesting Solutions LLC; ²Air Force Research Laboratory; ³UES, Inc.

9:30 AM

In-situ Micro-tensile Testing of Proton-irradiated HT-9 Steels: Tanvi Ajantiwalay¹; Stuart Maloy²; Khalid Hattar³; Assel Aitkaliyeva¹; ¹University of Florida; ²Los Alamos National Laboratory; ³Sandia National Laboratory



9:50 AM

Dislocation Structure in FeCrAl Alloys through Advanced In-situ Microscopy Experiments: Keyou Mao¹; Maxim Gussev¹; Caleb Massey¹; Kinga Unocic¹; Yukinori Yamamoto¹; Kevin Field²; Philip Edmondson¹; ¹Oak Ridge National Laboratory; ²University of Michigan

10:10 AM

In-situ Nanomechanics of Ni-based Superalloys and Bond Coating at Room **Temperature to 1000C**: *Sanjit Bhowmick*¹; Eric Hintsala¹; Praveena Manimunda¹; Douglas Stauffer¹; ¹Bruker

10:30 AM

Analysis of Deformation Mechanisms in Advanced FeCrAl Alloy via SEM-EBSD Insitu Testing: Nitish Bibhanshu¹; Maxim Gussev¹; Caleb Massey¹; Kevin Field²; ¹Oak Ridge National Laboratory; ²University of Michigan

10:50 AM

MEMS-based In-situ Tensile Experiments Designed to Arrest Catastrophic Failure inBrittleNanomaterials:DaehyeokAhn¹;DongchanJang²;¹KoreaAdvancedInstitute of Science & Technology; ²Korea Advanced Institute of Science & Technology

11:10 AM

In-situ Characterization of the Damage Initiation and Evolution in Sustainable **Cellulose-based Cottonid**: *Ronja Scholz*¹; Alexander Delp¹; Frank Walther¹; ¹TU Dortmund University

MATERIALS DESIGN

Metal-Matrix Composites: Advances in Analysis, Measurement and

Observations – Novel Composites and Coatings

- VEBSITE TMS

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Srivatsan Tirumalai, The University of Akron; William Harrigan, Gamma Alloys; Simona Hunyadi Murph, Savannah River National Laboratory

Tuesday AM March 16, 2021

Session Chair: William Harrigan, GAMMA Technology

8:30 AM Invited

Use of an Infrared Spectroscopic Method for Isotopic Analysis of Gaseous **Uranium Hexafluoride**: *K. Alicia Strange Fessler*¹; Patrick O'Rourke¹; Nicholas DeRoller¹; Darrell Simmons²; Steven Serkiz³; ¹Savannah River National Laboratory; ²Oak Ridge National Laboratory; ³Clemson University

9:00 AM

Recent Advances in Analysis, Measurement and Properties of Composite Metal Foams: Afsaneh Rabiei¹; Brian Lattimer²; Elias Bearinger²; ¹North Carolina State University; ²Virginia Tec

9:20 AM Invited

Effect of Heat Treatment on the Mechanical Properties of an Aluminum Alloy and Aluminum Alloy Composite: A Comparative Study: Shaik Mozammil¹; Jimmy Karloopia¹; Pradeep Jha¹; *Srivatsan Tirumalai*²; ¹Indian Institute of Technology Roorkee; ²University of Akron



9:50 AM Invited

2D Interlayer Enabled Electrical Ductility for Flexible Electronics: *Pilgyu Kang*¹; Chullhee Cho²; Amir Taqieddin²; Yuhang Jing²; Keong Yong²; Jin Myung Kim²; Md Farhadul Haque²; Narayana R. Aluru²; SungWoo Nam²; ¹George Mason University; ²University of Illinois at Urbana-Champaign

10:20 AM

A Method for Measuring Total Protium and Total Deuterium in a Gas Mixture Containing Hydrogen, Deuterium and Hydrogen Deuterium Mixture Using Gas Chromatography: Henry Sessions, Jr.1; Simona Hunyadi Murph²; ¹University of Georgia; ²Savannah River National Laboratory; University of Georgia

10:40 AM Iron Oxide - Gold Composite Nanoparticles and Nanogap Junctions for Sensing Applications Using Surface Enhanced Raman Scattering: Simona Hunyadi *Murph*¹; Emily Searles²; ¹Savannah River National Laboratory; University of Georgia; ²Savannah River National Laboratory

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — Hydormetallurgy I



Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

March 16, 2021 **Tuesday AM**

8:30 AM

Alkaline Leaching of Nickel from Electric Arc Furnace Dust Using Ammoniaammonium Glutamate as Lixiviant: Erik Prasetyo¹; ¹Indonesian Institute of Sciences

8:50 AM

Chemical Leaching of Inactive Gold Mine Tailings as Secondary Source of Cobalt and Nickel – A Preliminary Case Study: Marouen Jouini¹; Lucie Coudert¹; Mathilde Perrin²; ¹UQAT; ²Université de Lorraine

9:10 AM

Microbial Leaching for Recovery of Nickel & Cobalt from Lateritic Ore, A Review: Lala Behari Sukla¹; Archana Pattanaik¹; DP Krishna Samal¹; Debabrata Pradhan; ¹Siksha 'O' Anusandhan



MOBILE-FRIEND

9:30 AM Sulfuric Acid Leaching for Low-nickel Matte under Atmospheric Pressure: Wanhai Xiao¹; *Fenglong Sun*¹; Xuheng Liu¹; Zhongwei Zhao¹; ¹Central South University

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Microstructure and **Precipitation**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

March 16, 2021 **Tuesday AM**

Session Chairs: Thomas Voisin, Lawrence Livermore National Laboratory; Kaila Bertsch, Lawrence Livermore National Laboratory

8:30 AM

Chemistry Effects on a' Precipitation in FeCrAl Alloys: Andrew Hoffman¹; Soumya Nag¹; Chen Shen¹; Chao Jiang²; Yongfeng Zhang³; Raul Rebak¹; ¹GE Research; ²Idaho National Lab; ³University of Wisconsin-Madison



8:50 AM

Effect of Slip and Twinning Microstructure on High Pressure Phase Transformation in Zirconium: Mariyappan Arul Kumar¹; Yanbin Wang²; Rodney McCabe¹; Laurent Capolungo¹; Carlos Tome¹; ¹Los Alamos National Laboratory; ²Argonne National Laboratory

9:10 AM

Probing the Plasticity and Microstructure Evolution of an Icosahedral Quasicrystal i-Al-Pd-Mn at Elevated Temperatures

: Yu Zou¹; ¹University of Toronto

9:30 AM

Spinodal Decomposition in a Nanostructured Cu-Ti Alloy: Julian Rosalie¹; Oliver Renk²; ¹University of Leoben, Austria; ²Erich Schmid Institute, Austrian Academy of Sciences

9:50 AM

The Synergistic Role of Mn and Zr/Ti in Producing '/L1, Co-precipitates in Al-Cu Alloys: Jonathan Poplawsky¹; Brian Milligan²; Patrick Shower³; Lawrence Allard¹; Matthew Chisholm¹; Dongwon Shin¹; Amit Shyam¹; ¹Oak Ridge National Laboratory; ²Colorado School of Mines; ³GE Global Research

10:10 AM

Understanding the Influence of Thermal Gyrations on Solid-solid Interfaces in Ti-6Al-4V during EBM PBF Process Using In Situ TEM: Sriram Vijayan¹; Meiyue Shao¹; Joerg Jinschek¹; ¹The Ohio State University

10:30 AM

Variability of Grain Boundary Migration Behaviors among the Metastable Grain



TUESDAY AM

ONTENTS

TABLE

P

Boundary Structures: *Eric Homer*¹; Darcey Britton¹; Oliver Johnson¹; Lydia Serafin¹; Gus Hart¹; ¹Brigham Young University

NANOSTRUCTURED MATERIALS

Plasmonics in Nanocomposite Materials — From Theory to Application Session

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee

Program Organizers: Nasrin Hooshmand, Georgia Institute of Technology; Simona Hunyadi Murph, Savannah River National Laboratory; Mahmoud Abdelwahed, The University of Texas at San Antonio

Tuesday AM March 16, 2021

Session Chair: Simona Hunyadi Murph, Savannah River National Laboratory (SRNL)

8:30 AM Keynote **Nanoplasmonics and Its Applications in Nanomedicine**: *Mostafa El-Sayed*¹; ¹Georgia Institute of Technology

9:15 AM Invited Fin p-n Heterojunctions for High Brightness Light Emitting Diodes and Lasers at Sub-micron Scale: Babak Nikoobakht¹; Robin Hansen²; Yuqin Zong²; Amit Agrawal²; Michael Shur³; Jerry Tersoff⁴; ¹National Institute of Standards and Technology; ²NIST; ³Rensselaer Polytechnic Institute; ⁴IBM T. J. Watson Research Center



8:30 AM Synthesis of Chicken Feather Fiber Bio-waste Derived Sustainable Nitrogen

9:45 AM Invited Spectral Enhancement of Dye Molecules Adsorbed on Titania Prepared on Gold Nanoparticles: *Hiromasa Nishikiori*¹; Yosuke Kageshima¹; Katsuya Teshima¹; ¹Shinshu University

10:05 AM Invited Engineered Plasmonic Nanoparticle Based Detection: Advanced Sensitivity and **Selectivity**: *Nasrin Hooshmand*¹; ¹Georgia Institute of Technology

ENERGY & ENVIRONMENT

Powder Materials for Energy Applications – Novel Powder Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Powder Materials Committee**

Program Organizers: Kathy Lu, Virginia Polytechnic Institute and State University; Eugene Olevsky, San Diego State University; Hang Yu, Virginia Polytechnic Institute and State University; Ruigang Wang, The University of Alabama; Isabella Van Rooyen, Idaho National Laboratory

Tuesday AM March 16, 2021

Session Chair: Kathy Lu, Virginia Polytechnic Institute and State University

TABLE **NTENTS P**





TUESDAY AM

Doped-carbon Material: Vijaya Rangari¹; *Zaheeruddin Mohammed*¹; Zahria Duncan¹; Shaik Jeelani¹; ¹Tuskegee University

8:50 AM Invited Mechanical Activation Enhanced Solid-state Synthesis of NaCrO2 Cathode Material for Na-ion Batteries: Leon Shaw¹; Mei Luo¹; Angel Ortiz²; ¹Illinois Institute of Technology; ²Universidad de Extremadura

9:20 AM Invited **Powder to Energy Application**: Jung Pyung Choi¹; John Hardy¹; ¹Pacific Northwest National Laboratory

9:50 AM Invited **PowderCharacteristicsofPerovskiteAnodesontheElectrochemicalPerformance** of Solid Oxide Fuel Cell: A Perspective: Manoj Mahapatra¹; ¹University of Alabama at Birmingham

10:20 AM Structural Evolution and Electrical Conductivity of Ti3C2-SiOC Systems: Kathy Lu¹; *Sanjay Kumar*¹; ¹Virginia Polytechnic Institute and State University

MATERIALS PROCESSING

Rare Metal Extraction & Processing – REEs



Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

March 16, 2021 **Tuesday AM**

8:30 AM Keynote **Innovative Reactors for Recovery of Rare Earth Elements (REE)**: Alison Lewis¹; Jemitias Chivavava¹; Jacolien DuPlessis¹; Dane Smith¹; Jody-Lee Smith¹; ¹University of Cape Town

8:50 AM Invited Study of the Recovery of Rare Earth Elements from Ion Adsorption Clays through **Perolation Leaching Processes**: *Jochen Petersen*¹; Megan Becker²; Chad Naude²; ¹University of Cape Town; ²Univ of Cape Town

9:10 AM

Recovery of Rare Earth Elements from Recycled Hard Disk Drive Mixed Steel and Magnet Scrap: Tedd Lister¹; Michelle Meagher²; *Mark Strauss*¹; Luis Aldana¹; Harry Rollins¹; ¹Idaho National Laboratory; ²Colorado School of Mines

9:30 AM Invited **Extraction Chromatography for Separation of Rare Earth Elements**: *Meher Sanku*¹; Kerstin Forsberg¹; Michael Svärd¹; ¹KTH Royal Institute of Technology



MOBILE-FRIENDL

9:50 AM Invited

Tool and Workflow for Systematic Design of Reactive Extraction for Separation and Purification of Valuable Components: Hana Benkoussas¹; David Leleu¹; Swagatika Satpathy¹; Zaheer Shariff¹; *Andreas Pfennig*¹; ¹University of Liège

10:10 AM Invited **Rethinking Mineral Processing and Extractive Metallurgy Approaches to Ensure** a Sustainable Supply of High-tech and Critical Raw Materials: Yousef Ghorbani¹; Glen Nwaila²; Steven Zhang³; Jan Rosenkranz¹; ¹Luleå University of Technology; ²University of the Witwatersrand; ³PG Techno Wox, 43 Patrys Avenue, Helikon Park

10:30 AM Invited

Extraction of Rare Earth Metals: The New Thermodynamic Considerations towards Process Hydrometallurgy: Ajay Patil¹; Rudolf Struis¹; Andrea Testino²; Christian Ludwig¹; ¹Paul Scherrer Institut and École Polytechnique Fédérale de Lausanne; ²Paul Scherrer Institut

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture in **Complex Materials**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

Tuesday PM March 16, 2021

Session Chair: Neville Moody, Sandia National Laboratories - Retired

2:00 PM Invited Fracture Resistance of Hierarchical Metallic Nanocomposite Thin Films: *Amit Misra*¹; Y. Cui¹; B. Derby¹; N. Li²; ¹University of Michigan; ²LANL

2:40 PM

In-situFracturealongDistinctInterfaceTypes:*MichaelBurtscher*¹;MarkusAlfreider¹; MichaelWurmshuber²; Klemens Schmuck¹; Helmut Clemens³; Svea Mayer¹; Daniel Kiener¹; ¹Montanuniversität Leoben, Austria; ²Department Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Austria; ³Department Materials Science, Chair of Physical Metallurgy and Metallic Materials, Montanuniversität Leoben, Austria

3:00 PM

TheClampedBeamBendingasaLengthScaleCompatibleFractureTestGeometry: *Balila Nagamani Jaya*¹; Ashwini Kumar Mishra¹; Hrushikesh Sahasrabuddhe¹; Neha Kumari¹; Deepesh Yadav¹; Tanmayee More¹; Tejas Chaudhari¹; ¹Indian Institute of Technology Bombay

3:20 PM

A Griffith's Theory-based Model for Strength of Silicon Nitride Nanoporous Membranes from Atomistic Simulation Perspective: *Ali Khourshaei Shargh*¹; Gregory Madejski¹; James McGrath¹; Niaz Abdolrahim¹; ¹University of Rochester

3:40 PM Invited Transformation-induced Cracking in ZrO₂ Shape-memory Ceramics: towards Cyclic Stability in Polycrystals: *Edward Pang*¹; Isabel Crystal¹; Christopher Schuh¹; ¹Massachusetts Institute of Technology

SPECIAL TOPICS

2021 Institute of Metals Lecture/Robert Franklin Mehl Award — 2021 Institute of Metals Lecture/Robert Franklin Mehl Award

Tuesday PM March 16, 2021

12:00 PM

Introduction of Award Recipient: 2021 Institute of Metals Lecture/Robert Franklin Mehl Award: James Williams¹; ¹The Ohio State University

12:05 PM Keynote New Superalloys in the Co-Ni Design Space: *Tresa Pollock*¹; ¹University of California, Santa Barbara

12:45 PM Question and Answer Period Moderator: Jim Williams, The Ohio State

TMS





TUESDAY PM

SPECIAL TOPICS

2021 TMS Special Sessions — EPD/MPMD Awards Ceremony & Special Lecture

March 16, 2021 **Tuesday PM**

12:00 PM **EPD Awards Ceremony**: Christina Meskers

12:30 PM MPMD Awards Ceremony & Introduction of Special Lecturer: Edward Glaessgen¹; ¹NASA Langley Research Center

12:45 PM MPMD Special Lecturer: Qualification and Certification Strategies for Additive Manufactured Parts for Manned Spaceflight: Richard Russell¹; ¹NASA Kennedy **Space Center**

SPECIAL TOPICS

2021 TMS Special Sessions — LMD Awards Ceremony & Special Lecture

Tuesday PM March 16, 2021

12:00 PM

Π

LMD Awards Ceremony: Eric Nyberg¹; ¹Tungsten Heavy Powder & Parts

12:30 PM LMD Scholarship Lecturer: Zachary Wolff¹; ¹University of Nevada Reno

12:40 PM LMD Special Lecturer Introduction: Eric Nyberg¹; ¹Tungsten Heavy Powder & Parts

12:45 PM LMD Special Lecturer: Near Net Manufacturing of Light Metal Alloys: Mark Easton¹; ¹RMIT University

SPECIAL TOPICS

2021 TMS Special Sessions — Student Career Forum

Tuesday PM March 16, 2021

2:00 PM **Student Career Forum**

SPECIAL TOPICS

2021 TMS Special Sessions — Young Professional Tutorial Lecture

March 16, 2021 **Tuesday PM**

12:00 PM

Young Professional Tutorial Lecture Introduction: Abby Cisko¹; ¹US Army ERDC

MOBILE-FRIEND

12:05 PM

Early Career Faculty Fellow Recipient: Electrochemical Healing of Metals: A New Way to Repair Additive and Cellular Metals at Room Temperature: James Pikul¹; ¹University of Pennsylvania

12:35 PM Early Career Faculty Fellow Recipient: Integrated Computational Materials **Design for Alloy Additive Manufacturing**: *Wei Xiong*¹; ¹University of Pittsburgh

ADVANCED MATERIALS

2D Materials – Preparation, Properties & Applications – Modeling & **Simulations I**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Sufian Abedrabbo, Khalifa University; Amber Shrivastava, Indian Institute of Technology Bombay

Tuesday PM March 16, 2021

Session Chairs: Gerald Ferblantier, University of Strasbourg; Sufian Abedrabbo, Khalifa University



TUESDAY PM

AB

Π

P

ONTENTS

2:00 PM

Computational Synthesis of 2D Materials: A High-throughput Approach to Materials Design: Tara Boland¹; Arunima Singh¹; ¹Arizona State University

2:20 PM Invited Assessment of Gas Sensing Properties of 2D Materials by Comprehensive Density **Functional Theory Calculations**: Siby Thomas¹; *Mohsen Asle Zaeem*¹; ¹Colorado School of Mines

2:45 PM Invited Computational Modeling of Two-Dimensional Materials for Sustainable Energy **Storage**: *Dibakar Datta*¹; ¹New Jersey Institute of Technology

3:10 PM Invited Thermal Laser Assisted Manufacturing of Two-dimensional Atomic Layers Heterostructures: Yingtao Wang¹; Xian Zhang¹; ¹Stevens Institute of Technology

3:35 PM Invited

Energetics and Electronic Properties of Dopants and Defect Complexes in **2D Transition Metal Dichalcogenides from First-principles**: Anne Marie Tan¹; Christoph Freysoldt²; *Richard Hennig*¹; ¹University of Florida; ²Max-Planck-Institut f "ur Eisenforschung GmbH

4:00 PM Invited Stabilization of a Ferroelectric Phase in Two Dimensional MXene Monolayers: Joshua Young¹; Mo Li¹; Olamide Omisakin¹; ¹New Jersey Institute of Technology

4:25 PM Invited

Tracking Structural Flexibility and Dynamics in 2D Metal-Organic Frameworks and their Effects on Electrical Conductivity and Catalytic Activity: Farnaz Shakib¹; Mohammad Momeni¹; ¹New Jersey Institute of Technology



NUCLEAR MATERIALS

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — High Throughput Testing, Advanced Characterization and Property Measurement

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Tuesday PM March 16, 2021

Session Chairs: Janelle Wharry , Purdue University ; Tiankai Yao, Idaho National Laboratory

2:00 PM Invited A Standards Perspective on Nanomechanical Testing to Accelerate Nuclear Materials Development & Qualification: *Janelle Wharry*¹; Priyam Patki¹; George Warren¹; Patrick Warren¹; J Hall²; ¹Purdue University; ²Westinghouse Electric Company, LLC



2:30 PM

A Rapid Turnaround Approach Studying Helium Effects in Materials: Peter Hosemann¹; Andrew Scott¹; Sarah Stevenson¹; Mehdi Balooch¹; ¹University of California Berkeley

2:50 PM

High-throughput Heavy Ion Irradiation of CrFeMnNi Magnetron-sputtered Combinatorial Thin Film: *Calvin Parkin*¹; Michael Moorehead¹; Mohamed Elbakhshwan¹; Kumar Sridharan¹; Chuan Zhang²; Alan Savan³; Alfred Ludwig³; Adrien Couet¹; ¹University of Wisconsin Madison; ²Computherm, LLC; ³Ruhr-Universität Bochum

3:10 PM

Accelerated Study of Thermal and Irradiation Creep in Fe-based Multi-principal Element Alloys: *Marcus Parry*¹; Colin Judge²; Cheng Sun²; Wen Jiang²; Boopathy Kombaiah²; Gary Was³; Jeffery Aguiar²; Taylor Sparks¹; ¹University of Utah; ²Idaho National Laboratory; ³University of Michigan

3:30 PM

High-temperature, High-throughput Ion Irradiation Enabled by Additive Technologies: *Michael Moorehead*¹; Calvin Parkin¹; Phalgun Nelaturu¹; Michael Niezgoda¹; Mohamed Elbakhshwan¹; Kumar Sridharan¹; Dan Thoma¹; Adrien Couet¹; ¹University of Wisconsin - Madison

3:50 PM

In-situ TEM Heating Chip Experiments to Study Thermal Behavior of U-Zr Metallic Fuel: *Tiankai Yao*¹; Fei Teng¹; Daniel Murray¹; Jlan Gan¹; Michael Benson¹; Lingfeng He¹; ¹Idaho National Laboratory

4:10 PM

Multiscale Characterization of Defects in Ion Irradiated Ceramics for Validation of Atomistic Models: *Marat Khafizov*¹; Vinay Chauhan¹; Lingfeng He²; Janne Pakarinen³; David Uurley², ¹Obie State University ²Idaha National Laboratory ³Studeyild

David Hurley²; ¹Ohio State University; ²Idaho National Laboratory; ³Studsvik

CONTENTS TABLE Q

4:30 PM In-situ Thermal Conductivity Measurement of SiC Composite: Di Chen¹; Wei-Kan Chu¹; Piyush Sabharwall²; ¹University of Houston; ²Idaho National Laboratory

SPECIAL TOPICS

Acta Materialia Symposium — Acta Materialia Award Session

Program Organizer: Carolyn Hansson, University of Waterloo

March 16, 2021 **Tuesday PM**

2:00 PM

IntroductoryComments:ActaMaterialiaSymposium:CarolynHansson¹;¹University of Waterloo

2:05 PM Invited Acta Materialia Gold Medal Lecture: Modeling Microstructure Complexity for **Better Property Predictions**: *Günter Gottstein*¹; ¹RWTH Aachen University

2:25 PM Invited Acta Materialia Silver Medal Lecture: Measuring Hydrogen in Steels by Using **Atom Probe Tomography**: *Julie Cairney*¹; ¹The University of Sydney

2:45 PM Invited

Acta Materialia Hollomon Materials and Society Award: Global Energy Challenges and Development of Thermoelectric Materials and Systems in China: Qingjie *Zhang*¹; ¹Wuhan University of Technology



TUESDAY PM

3:05 PM Invited Acta Materialia Mary Fortune Global Diversity Lecture: STEM Mentor Programs and New Opportunities for Women and Other Under- Represented Groups in the Materials Science: Katalin Balazsi¹; ; ¹Centre for Energy Research

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Inconel, New Alloys, and **Functional Gradients**

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Tuesday PM March 16, 2021

Session Chair: Mohsen Seifi, ASTM International/Case Western Reserve University

2:00 PM Invited

Laser Powder Bed Fusion of TiTa Alloys: Process Optimisation and Fatigue **Properties**: Andrey Molotnikov¹; Erin Brodie²; Thomas Niendorf³; ¹RMIT University,

Centre for Additive Manufacturing; ²Monash University; ³University of Kassel

2:30 PM

Synchrotron Imaging of the Influence of TiB2 in Suppressing Hot Cracking during Laser Powder Bed Fusion of Al-2139: *David Rees*¹; Chu Lun Alex Leung¹; Joe Elambasseril²; Sebastian Marussi¹; Saurabh Shah¹; Shashidhara Marathe³; Milan Brandt²; Mark Easton²; Peter Lee¹; ¹University College London; ²RMIT University; ³Diamond Light Source Ltd

2:50 PM

Microstructural Heterogeneity and Mechanical Anisotropy of 18Ni-330 Maraging Steel Fabricated by Selective Laser Melting: The Effect of Build Orientation and Height: Yao Yi¹; Kaiwen Wang²; *Xiaoqing Wang*³; Lin Li¹; Wenjun Cai²; Samuel Kelly³; Natalia Esparragoza³; Matthew Rosser³; Feng Yan¹; ¹The University of Alabama; ²Virginia Polytechnic Institute and State University; ³Jacksonville State University

3:10 PM

Characterization of 3D-printed Metals with Ultrasonic Technique: *Terence Costigan*¹; Ping-Chuan Wang¹; Robert Van Pelt²; Aaron Nelson¹; ¹SUNY New Paltz; ²Sono-Tek Corporation

3:30 PM Invited

Tensile and Fatigue Behavior of Cold Sprayed Material Using Heat Treated Feedstock Powders: *Luke Brewer*¹; A. R. Webb¹; Ning Zhu¹; J. Brian Jordon¹; ¹The University of Alabama

ADDITIVE TECHNOLOGIES

Additive Manufacturing for Energy Applications III — Modeling and NondestructiveTesting in Additive Manufacturing



Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Nuclear Materials Committee

Program Organizers: Isabella Van Rooyen, Idaho National Laboratory; Indrajit Charit, University of Idaho; Subhashish Meher, Idaho National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Kumar Sridharan, University of Wisconsin-Madison; Xiaoyuan Lou, Auburn University

Tuesday PM March 16, 2021

Session Chair: Xiaoyuan Lou, Auburn University

2:00 PM Invited Porosity in Metal Additive Manufacturing: X-ray Tomography Insights: Anton du Plessis¹; ¹Research Group 3D Innovation, Stellenbosch University

2:20 PM

Effects of Void Configuration on the Overall Thermal and Mechanical Behavior of Porous Materials: A Numerical Modeling Approach: *Yu-lin Shen*¹; Mohammad Abdo²; Binh Pham²; Isabella Van Rooyen²; ¹University of New Mexico; ²Idaho National Laboratory

2:40 PM

Experimental and Numerical Investigation of Single Clads Generated by Directed Energy Deposition Additive Manufacturing Processes: *Luis Nunez*; John Shelton¹; Kyu Cho¹; ¹Northern Illinois University

3:00 PM

Multi-scale Multi-fidelity Metamodeling for Advanced Materials: Mohammad

*Abdo*¹; Yu-Lin Shen²; Cam Pham¹; Isabella Von Rooyen¹; ¹Idaho National Laboratory;

²University of New Mexico

3:20 PM

Detection of Defects in Additively Manufactured Metals Using Thermal **Tomography**: *Alexander Heifetz*¹; Dmitry Shribak¹; Zoe Fisher¹; William Cleary²; ¹Argonne National Laboratory; ²Westinghouse Electric Company

3:40 PM

Real Time Non-destructive Evaluation during 3D Manufacturing of Metal Parts: Araz Yacoubian¹; ¹LER Technologies, Inc.

4:00 PM

Combining Modelling and Microstructural Studies in Explaining the Laser Parameter Effect on Superalloy Cracking during Selective Laser Melting: Marcus Lam¹; ¹Monash University

4:20 PM

Simulation of Part Printability in Electron Beam Melting Additive Manufacturing: *Yousub Lee*¹; Patxi Fernandez-Zelaia¹; Srdjan Simunovic¹; Mike Kirka¹; ¹Oak Ridge National Laboratory

4:40 PM

Defect Analysis in Selectively Laser Melted Parts via Surface Topography **Characterization**: *Qingyang Lu*¹; Matteo Seita¹; ¹Nanyang Technological University

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Metals: Applications of Solidification Fundamentals - Solidification Structure and Defects



TUESDAY PM

CONTENTS

TABLE OF

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Solidification Committee

Program Organizers: Alex Plotkowski, Oak Ridge National Laboratory; Lang Yuan, University of South Carolina; Kevin Chaput, Northrop Grumman; Mohsen Asle Zaeem, Colorado School of Mines; Wenda Tan, University of Utah; Lianyi Chen, University of Wisconsin-Madison

Tuesday PM March 16, 2021

2:00 PM

A Phase-field Study of Epitaxial Effect on Solidification Microstructure in Metal Additive Manufacturing: *Jiwon Park*¹; Joo-Hee Kang¹; Chang-Seok Oh¹; ¹Korea Institute of Materials Science

2:20 PM

Composition and Equilibrium Phase Diagram Feature Effects on the Printability of Alloys: Raiyan Seede¹; Xueqin Huang¹; Bing Zhang¹; Austin Whitt¹; Alaa Elwany¹; Raymouno Arroyave¹; Ibrahim Karaman¹; ¹Texas A&M University

2:40 PM

Influence of Process Parameters on the Microstructure Evolution and Mechanical **Properties of Additively Manufactured 316L Stainless Steel**: Ankur Kumar Agrawal¹; Dan Thoma¹; ¹University of Wisconsin Madison

3:00 PM

LPBF Processing of the Al-Ni Eutectic Alloy: Experiments and Phase Field **Simulations**: *Guillaume Boussinot*¹; Markus Apel¹; Markus Döring²; ¹Access e.V.; ²LPT University Erlangen



Additive Manufacturing: Materials Design and Alloy Development III -- Super Materials and Extreme Environments — High Temperature and Heavy Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

3:20 PM

Modeling Grain Refinement for Metallic Additive Manufacturing: Yijia Gu^{1} ; ¹Missouri University of Science and Technology

3:40 PM

New Composition Based Index for Solidification Cracking Resistance: Rafael *Giorjao*¹; Benjamin Sutton¹; Antonio Ramirez¹; ¹The Ohio State University

4:00 PM

Phase-Field Modeling of CET During Alloy Solidification: An Insight for Additive Manufacturing: Nima Najafizadeh¹; Yijia Gu¹; ¹University of Missouri Science and Technology

4:20 PM

Quantifying the Influence of Local Layer Thickness on Pore Evolution during Laser Powder Fusion Using High-speed X-ray Imaging: Chu Lun Alex Leung¹; Yuze Huang¹; Samuel J. Clark¹; Yunhui Chen¹; Sebastian Marussi¹; Lorna Sinclair¹; Iain Todd²; Margie P. Olbinado³; Elodie Boller⁴; Alexander Rack⁴; Peter D. Lee¹; ¹University College London; ²University of Sheffield; ³Paul Scherrer Institute; ⁴European Synchrotron Radiation Facility

ADDITIVE TECHNOLOGIES



TABLE OF

TUESDAY PM

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek Innovations LLC

Tuesday PM March 16, 2021

Session Chair: Atieh Moridi, Cornel

2:00 PM

Process Development for the Selective Laser Melting of Tungsten Carbide-nickel Matrix Composites: Edgar Mendoza Jimenez¹; Baby Reeja-Jayan¹; Jack Beuth¹; ¹Carnegie Mellon University

2:20 PM

Laser Powder-bed Fusion Austenitic Steels with Superior Creep Resistance: Sebastien Dryepondt¹; Peeyush Nandwana¹; Kinga Unocic¹; Patxi Fernandez-Zelaia¹; Ying Yang¹; Rangasayee Kannan¹; Yousub Lee¹; Fred List¹; ¹Oak Ridge National Laboratory

2:40 PM

Development of Multi-principle Element Alloys for Oxidation Resistant Coatings Applied with Additive Manufacturing: Jose Loli¹; Yining He¹; Amish Chovatiya¹; Zachary Ulissi¹; Bryan Webler¹; Maarten De Boer¹; Jack Beuth¹; ¹Carnegie Mellon University

3:00 PM

Reactive Selective Laser Synthesis and Additive Manufacturing of Ultra-high **Temperature Ceramics**: *Adam Peters*¹; Dajie Zhang²; Alberto Hernandez¹; Michael

Brupbacher²; Dennis Nagle¹; Tim Mueller¹; James Spicer¹; ¹Johns Hopkins University;

²The Johns Hopkins Applied Physics Laboratory

3:20 PM

The Mechanisms Behind the Effect of Oxygen on DED AM Ti Alloy Build: Caterina *Iantaffi*¹; Yunhui Chen¹; Samuel J. Clark¹; Robert C. Atwood²; Eral Bele¹; Martina Meisnar³; Thomas Rohr⁴; Lertthanasarn Jedsada⁵; Minh-Son Pham⁵; Peter D. Lee¹; ¹UCL Mechanical Engineering; ²Diamond Light Source Ltd; ³ESA-RAL Advanced Manufacturing Laboratory; ⁴ESA-ESTEC; ⁵Imperial College London

3:40 PM

A Novel Heat Treatment Design to Overcome Inferior Creep Behaviour of SLM **Processed IN738LC Alloy**: *Haoyu Song*¹; ¹MCAM, Monash University

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Ni-based Superalloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, **TMS: Shaping and Forming Committee**

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

MOBILE-FRIEND

Tuesday PM March 16, 2021

Session Chairs: Katerina Christofidou, The University of Sheffield; Chantal Sudbrack, National Energy Technology Laboratory

2:00 PM Invited

Impact of Post-processing on the Performances of Laser Additively Manufactured **High-** γ ' **Ni Superalloys**: *Ning Zhou*¹; Austin Dicus¹; Stephane Forsik¹; Tao Wang¹; Gian Colombo¹; Mario Epler¹; ¹Carpenter Technology

2:30 PM

Improving the Creep Properties on gamma prime-strengthened Nickel-based Superalloy by Selective Laser Melting: Marcus Lam¹; ¹Monash University

2:50 PM

New Superalloy ABD-900AM for Additive Manufacturing: The Role of Heat Treatment on Mechanical Properties: Yuanbo Tang¹; Joseph Ghoussoub¹; John Clark²; Andre Nemeth²; Roger Reed¹; ¹University of Oxford; ²OxMet Technologies

3:10 PM

Microstructure and Texture Evolution During Printing and Post Processing of Nibased Superalloy: Colleen Hilla¹; Wei Zhang¹; Michael Mills¹; Alber Sadek²; Hyeyun Song³; ¹The Ohio State University; ²Edison Welding Institute ; ³Edison Welding Institute

3:30 PM Invited

Applying Additive Manufacturing Itself as a High-throughput Tool to Accelerate Heat Treatment Design of Additively Manufactured Alloys: Yunhao Zhao¹; Noah Sargent¹; Kun Li¹; *Wei Xiong*¹; ¹University of Pittsburgh



Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko

4:00 PM

Simulation of Solid State Precipitation during Post Process Annealing of Additively Manufactured alloy 625: Bala Radhakrishnan¹; Younggil Song¹; John Turner¹; ¹Oak **Ridge National Laboratory**

4:20 PM

Assessing Compositional Gradients in DED Inconel 718 Builds via Directional **Reflectance Microscopy**: *Ekta Jain*¹; Yeoh Yong Chen¹; Bernard Gaskey¹; Guido Macchi²; Antonio Mattia Grande²; Matteo Seita¹; ¹NTU Singapore; ²Politecnico di Milano, Italy

4:40 PM

Effect of Stress-relief Treatments on The Microstructure and Mechanical Response of Additively Manufactured IN625 Thin-walled Elements: Arunima Banerjee¹; Mo-Rigen He¹; William Musinski²; Paul Shade²; Marie Cox²; Edwin Schwalbach²; Kevin Hemker¹; ¹Johns Hopkins University; ²Air Force Research Laboratory

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation – Session IV**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**



TUESDAY PM

Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Tuesday PM March 16, 2021

2:00 PM Invited

A Framework for Quantitative Measurement of Plastic Deformation in Relation to 3D Microstructure: Jean-Charles Stinville¹; M. A. Charpagne¹; A. Cervellon¹; J. Hestroffer¹; M. P. Echlin¹; V. Valle²; D. Texier³; I.J. Beyerlein¹; T. M. Pollock¹; ¹University of California, Santa Barbara; ²Institut P' - UPR 3346, CNRS - Université de Poitiers - ENSMA; ³Institut Clément Ader - UMR CNRS 5312

2:30 PM

Characterization and Modelling of Twin Evolution and Cyclic Deformation in Magnesium Alloys by High Energy X-ray Diffraction Microscopy: Duncan Greeley¹; Mohammadreza Yaghoobi¹; Darren Pagan²; Veera Sundararaghavan¹; John Allison¹; ¹University of Michigan; ²Cornell High Energy Synchrotron Source

2:50 PM

Elastoplastic Transition in a Metastable 8-titanium Alloy, Timetal 18 by In-situ High Energy X-ray Diffraction: *Jishnu Bhattacharyya*¹; Sriramya Nair²; Darren Pagan³; Vahid Tari⁴; Ricardo Lebensohn⁵; Anthony Rollett⁶; Sean Agnew¹; ¹University of Virginia; ²Cornell University; ³Cornell High Energy Synchrotron Source, Cornell University; ⁴Eaton Corporate Research and Technology; ⁵Los Alamos National Laboratory; ⁶Carnegie Mellon University

3:10 PM

A Strain Gradient Crystal Plasticity Constitutive Model for Hexagonal Close-

packed Polycrystals: Omid Sedaghat¹; Hamidreza Abdolvand¹; ¹Western University

3:30 PM Estimating Stress on the Microstructural Length Scale Using the Measured Strain Field: Benjamin Cameron¹; Cem Tasan¹; ¹Massachusetts Institute of Technology

3:50 PM Invited

FFT-based Modeling of Strain Localization in Nano-metallic Laminates: Miroslav *Zecevic*¹; Ricardo Lebensohn¹; Thomas Nizolek¹; Rodney McCabe¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

4:20 PM

Dynamic Recovery Observed in Distinct Grains Within A Polycrystalline Nickelbased Superalloy During Cyclic High Temperature Loading via High Energy X-ray **Diffraction Microscopy**: Sven Gustafson¹; Darren Pagan²; Paul Shade³; Michael Sangid¹; ¹Purdue University; ²Cornell High Energy Synchrotron Source; ³Air Force **Research Laboratory**

4:40 PM

Statistical Assessment of Strain Localization in Inconel 718 Informed by Digital Image Correlation Coupled with 3D EBSD: Marie Charpagne¹; J.C. Stinville¹; Andrew Polonsky¹; McLean Echlin¹; Valery Valle²; Tresa Pollock¹; ¹University of California, Santa Barbara; ²P' Institute ENSMA Poitiers

5:00 PM

Analysis of Slip Transfer in Ti-5al-2.5 (Wt. %) at Two Temperatures in Comparison to Pure Aluminum: Chelsea Edge¹; *Thomas Bieler*¹; ¹Michigan State University

5:20 PM

Orientation, Pattern Center Refinement and Deformation State Extraction



TUESDAY PM

TABLE

P

NTENTS

through Global Optimization Algorithms: Chaoyi Zhu¹; Christian Kurniawan¹; Marcus Ochsendorf¹; Marc De Graef¹; ¹Carnegie Mellon University

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Coating **Technologies and Surface Structuring for Tools I**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

Tuesday PM March 16, 2021

Session Chairs: Karine Mougin, IS2M UHA; Heinz Palkowski, IMET

2:00 PM Invited

Investigations on the Process Stability of Dry Deep Drawing with Volatile Lubricants Injected through Laser-drilled Microholes: Gerd Reichardt¹; Manuel Henn²; Kim Riedmüller¹; Rudolf Weber²; Thomas Graf²; Mathias Liewald¹; Daniel Hemming³; Georg Umlauf⁴; Paul Reichle³; Jakob Barz⁴; Günter E.M. Tovar³; ¹Institute for Metal Forming Technology; ²Institut für Strahlwerkzeuge; ³Institute of Interfacial Process Engineering and Plasma Technology; ⁴Fraunhofer Institute for Interfacial Engineering and Biotechnology



2:30 PM

Laboratory-on-a Crystal for Multifunctional, Multiscale Testing of Thin Films: *Ilia Ivanov*¹; ¹Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

2:50 PM Keynote

Nanomanipulation and Nanolithography Experiments on Mono- and Multilayer MoS2 Surfaces: Enrico Gnecco¹; Alper Özogul¹; Felix Cassin¹; Roberto Guerra²; Andrey Turchanin¹; Franciszek Krok³; ¹Friedrich Schiller University Jena; ²University of Milan; ³Jagiellonian University Krakow

3:30 PM

Development of a Laboratory Test to Identify Permanent PVD Coatings to Minimize Lubricant Use during Forging: *Kester Clarke*; Trevor Kehe¹; Spencer Randell¹; Stephen Midson¹; ¹Colorado School of Mines

3:50 PM

Molten Aluminum Test for the Identification of PVD Coating Candidates for Lubefree Aluminum Die Casting: *Nelson Delfino de Campos Neto*¹; Andras Korenyi-Both¹; Stephen Midson¹; Michael Kaufman¹; ¹Colorado School of Mines

ADVANCED MATERIALS

Advanced High Strength Steels V — Session IV

Sponsored by: TMS Structural Materials Division, TMS: Steels Committee

Program Organizers: Ana Luiza Araujo, CBMM North America Inc.; Louis Hector, General Motors Global Technical Center; Igor Vieira, Nucor Steel; Lijia Zhao, ArcelorMittal USA; Krista Limmer, CCDC Army Research Laboratory; Jonah Klemm-Toole, Colorado School of Mines; Sebastien Allain, Institut Jean Lamour; MingXin Huang, University of Hong Kong



TUESDAY PM

TABLE OF

ONTENTS

Tuesday PM March 16, 2021

2:00 PM

A Novel Study on Plasticity Mechanisms during Yield Point Elongation in Medium Manganese Steels: *Poornachandra Satyampet*¹; Saurabh Kundu²; Prita Pant¹; ¹Indian Institute of Technology Bomaby, Mumbai.; ²Tata Steels

2:20 PM

Strain Path Effect on Martensitic Transformation in Medium Mn Steels: *Poornachandra Satyampet*¹; Saurabh Kundu²; Prita Pant³; ¹Indian Institute of Technology Bomaby, Mumbai.;²Tata Steels; ³Indian Institute of technology Bomaby, Mumbai.

2:40 PM

Static Recrystallization during Hot Deformation of HSLANb-Bearing Steels: Rami Almatani¹; Juha Uusitalo²; Anthony Deardo¹; ¹University of Pittsburgh; ²University of Oulu

3:00 PM

Correlation of Rolling Schedules, Mechanical Properties, and SCC Susceptibility of API X70 Steel: Anthony Roccisano¹; *Shahrooz Nafisi*¹; Douglas Stalheim²; Reza Ghomashchi¹; ¹University of Adelaide; ²DGS Metallurgical Solutions, Inc.

3:20 PM

High-resolution Digital Image Correlation Study of Plasticity and Damage at Lamellar Scales in Ferrite -- Pearlite Steel: *Tijmen Vermeij*¹; Johan Hoefnagels¹;

TMS

¹Eindhoven University of Technology



Advanced Magnetic Materials for Energy and Power Conversion Applications — Application of Advanced Soft Magnetic Materials in Power Electronics and Motors

Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

Tuesday PM March 16, 2021

Session Chair: Alex Leary, NASA Glenn Research Center

2:00 PM

Advances in Amorphous Core Technology for Loss Reduction in Distribution Transformers: *Eric Theisen*¹; ¹Metglas Inc.

2:20 PM

Magnetic Augmented Rotation System (MARS) – An Update: Nuggehalli Ravindra¹; Chimaobi Ibeh¹; *Tyler Brunstein-Ellenbogen*¹; Bilal Adra¹; Balraj Mani¹; Tiensee Chow²; ¹New Jersey Institute of Technology; ²ETD Inc. **MOBILE-FRIEND**

2:40 PM

Overview of Magnetic Component Design for Power Converters: *Richard Beddingfield*¹; Paul Ohodnicki²; ¹North Carolina State University; ²University of Pittsburgh

3:00 PM Invited

Permanent Magnet Biased Inductors for Power Systems Applications: *Mark Nations*¹; ¹North Carolina State University

3:30 PM The Effects of Stack Manufacturing Processes on the Magnetic Properties of Iron-Cobalt Alloys: *Natan Aronhime*¹; ¹Carpenter Technology

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Functional Materials for Energy I

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Tuesday PM March 16, 2021

Session Chairs: Jung Pyung Choi, Pacific Northwest National Laboratory; Peter Godart, Massachusetts Institute of Technology



2:00 PM

Assessment of Grain Boundary Composition on the Thermodynamics Structural **Properties in Concentrated Ceramic Oxides**: *Tara Boland*¹; Arunima Singh¹; Peter Rez¹; Peter Crozier¹; ¹Arizona State University

2:20 PM

A Novel and Practical Water-reactive Aluminum Fuel from Scrap: Peter Godart¹; Douglas Hart¹; ¹MIT

2:50 PM

Aging Behavior of Advanced Martensitic Steels for Next Generation Diesel Engine **Pistons**: *Dean Pierce*¹; Govindarajan Muralidharan¹; Larry Allard¹; Jon Poplawsky¹; Ercan Cakmak¹; Artem Trofimov¹; Hsin Wang¹; Allen Haynes¹; ¹Oak Ridge National Laboratory

3:10 PM

Breaking Atomic-level Ordering via Biaxial Strain in Functional Oxides: A DFT **Study**: *Kanishk Rawat*¹; Dilpuneet Aidhy¹; Dillon Fong²; ¹University of Wyoming; ²Argonne National Laboratory

3:30 PM

Direct Correlation of Anion Conductivity with Grain Boundary Defect Chemistry in Concentrated Oxide Solid Solutions: Hasti Vahidi¹; Shengquan Xuan¹; William *Bowman*¹; ¹University of California, Irvine

3:50 PM

Effect of Alloying Elements (Ni, Co) on Low Pt-transition Metals Nanowires for **Oxygen Reduction Electrocatalysts:** Jaeyoung Yoo¹; Youngtae Park¹; Changsoo Lee²; *Hyuck Mo Lee*¹; ¹KAIST; ²KIER



TUESDAY PM

CONTENTS

TABLE OF

4:10 PM

Electrochemical Behavior of Palladium in 1-Ethyl-3-Methylimidazolium Chloride Ionic Liquid: Wu Zhang¹; Batric Pesic²; ¹Shenyang Ligong University; ²University of Idaho

CHARACTERIZATION

Advanced Real Time Imaging — Energy & Biomaterials

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

Tuesday PM March 16, 2021

Session Chairs: Anna Nakano, USDOE National Energy Technology Laboratory; Jinichiro Nakano, USDOE National Energy Technology Laboratory



3:40 PM Invited

2:00 PM Invited

Ultrafast Synchrotron X-ray Imaging and Modelling of Multiphase Flow in Ultrasound Based Materials Processing: Ling Qin¹; *Jiawei Mi*¹; ¹University of Hull, UK

2:20 PM Invited

In-operando Non-invasive Optical Visualization of Battery Reactions and **Processes**: *Nian Liu*¹; ¹Georgia Institute of Technology

2:40 PM

In-operando Investigations of Refractory Materials Interacting with Ash/Slag from Mixed Feedstock Gasification: *Jinichiro Nakano*¹; Anna Nakano¹; Ömer Dogan¹; Matthew Lambert²; Dana Goski²; ¹U.S. Department of Energy National Energy Technology Laboratory; ²Allied Mineral Products, LLC

3:00 PM

Evaluating Amplitude Variation of Frequency Spectrum in Ultrasound Imaging by Through Transmission Method: Koushik Paul¹; Leila Ladani¹; ¹Arizona State University

3:20 PM

In-situ Analysis of Select Oxygen Carrier Materials under Chemical Looping **Combustion Conditions**: Anna Nakano¹; Jinichiro Nakano²; Ömer Dogan³; ¹U.S. Department of Energy National Energy Technology Laboratory/ Leidos Research SupportTeam;²U.S.Department of Energy National Energy Technology Laboratory/ Leidos Research Support Team ; ³U.S. Department of Energy National Energy Technology Laboratory

MOBILE-FRIEND



Synchronized High-speed Microscopy and Thermo-analytical Measurement for Sub-mm/sub-ms-scale Cathodic Behavior in Molten Salt Electrolysis: Shungo *Natsui*¹; Ryota Shibuya²; Hiroshi Nogami¹; Tatsuya Kikuchi²; Ryosuke Suzuki²; ¹Tohoku University; ²Hokkaido University

4:00 PM Break

4:20 PM Panel Discussion

MATERIALS PROCESSING

Advances in Powder and Ceramic Materials Science — Ceramic-based **Composites**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Materials Characterization Committee, TMS: Powder Materials Committee

Program Organizers: Bowen Li, Michigan Technological University; Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology; Kathy Lu, Virginia Polytechnic Institute and State University; Rajiv Soman, Eurofins EAG Materials Science LLC; Fagin Dong, Southwest University of Science and Technology; Jinhong Li, China University of Geosciences (Beijing); Ruigang Wang, The University of Alabama; Eugene Olevsky, San Diego State University

March 16, 2021 **Tuesday PM**

Session Chair: Dipankar Ghosh, Old Dominion University



2:00 PM

Low-cost Forming and Reactive Melt Infiltration Processing of High-temperature, Thermally-cyclable Carbide/Metal Composites in Complex, Near Net Shapes for Renewable Energy Applications: Yujie Wang¹; Priyatham Tumurugoti¹; Zhenhui Chen¹; Alex Strayer¹; Adam Caldwell¹; Saeed Bagherzadeh¹; Grigorios Itskos¹; Kevin Trumble¹; Mario Caccia¹; Kenneth Sandhage¹; ¹Purdue University

2:20 PM

Diamond Graphitization and Its Effect on Hardness of Diamond Particulate **Ceramic Composites**: Jerry LaSalvia¹; Anthony DiGiovanni¹; Kristopher Behler¹; William Shoulders¹; Scott Walck¹; ¹CCDC Army Research Laboratory

2:40 PM

Bulk High-entropy Nitrides and Carbonitrides: Olivia Dippo¹; Neda Mesgarzadeh¹; Tyler Harrington¹; Grant Schrader¹; Kenneth Vecchio¹; ¹University of California San Diego

MATERIALS DESIGN

Al/Data Informatics: Applications and Uncertainty Quantification at Atomistics and Mesoscales — Session IV

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid



Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Tuesday PM March 16, 2021

Session Chairs: Sukriti Manna, Argonne National Laboratory; Noah Paulson, Argonne National Laboratory

2:00 PM

Fast Crystal Structure Reconstruction and Prediction Method: Based on X-ray **Diffraction Dataset and Neural Network**: *Cheng-Che Tung*¹; Yan-Zhen Chen¹; Yuan-Yu Lin²; Nan-Yow Chen³; An-Cheng Yang³; Po-Yu Chen¹; ¹National Tsing Hua University; ²National Chiao Tung University; ³National Center for High-Performance Computing

2:20 PM

Finding and Sharing Atomistic Materials Data and Software with the NIST Materials **Resource Registry**: *Chandler Becker*¹; Raymond Plante¹; Laura Bartolo²; Robert Hanisch¹; James Warren¹; Gretchen Greene¹; ¹Material Measurement Laboratory, National Institute of Standards and Technology; ²Center for Hierarchical Materials Design, Northwestern University

2:40 PM

Accelerating High Throughput Materials Simulation Studies Using Machine Learning Based Application Programming Interface (API): Jason Gibson¹; Stephen Xie¹; Richard Hennig¹; ¹University of Florida

3:00 PM

Coupling Machine Learning and Global Structure Optimization in GASP 2.0: Stephen Xie¹; Shreyas Honrao¹; Venkata Kolloru¹; Richard Hennig¹; ¹University of



WEBSITE TMS Harnessing Materials Data and Simulation Capabilities for the Accelerated **Discovery of Photocathode Materials**: *Evan Antoniuk*¹; Yumeng Yue¹; Yao Zhou¹; Peter Schindler¹; W. Schroeder²; Theodore Vecchione³; Bruce Dunham⁴; Piero Pianetta³; Evan Reed¹; ¹Stanford University; ²University of Illinois at Chicago; ³SLAC; ⁴SLAC

3:40 PM

DeNovoDesignofTherapeuticAgentsAgainstCOVID-19UsingArtificialIntelligence: Srilok Srinivasan¹; Rohit Batra¹; Henry Chan¹; Ganesh Kamath²; Mathew Cherukara¹; Subramanian Sankaranarayanan¹; ¹Argonne National Laboratory; ²Dalzielfiver LLC

4:00 PM

Al Guided Discovery of Self-assembly Peptide Sequences using Monte Carlo Tree Search and Coarse-grained Simulations: Rohit Batra¹; Troy Loeffler¹; Henry Chan¹; Srilok Srinivasan¹; Christopher Fry¹; Subramanian Sankaranarayanan¹; ¹Argonne National Lab

MATERIALS DESIGN

AI/Data informatics: Design of Structural Materials — AI/ML for Design of **Structural Alloys & Additively Manufactured Materials**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee



MOBILE-FRIEND

Program Organizers: Jennifer Carter, Case Western Reserve University; Amit Verma, Carnegie Mellon University; Natasha Vermaak, Lehigh University; Jonathan Zimmerman, Sandia National Laboratories; Darren Pagan, Pennsylvania State University; Chris Haines, Ccdc Army Research Laboratory; Judith Brown, Sandia National Laboratories

Tuesday PM March 16, 2021

2:00 PM Invited Zoning Processing Spaces for Additive Manufacturing: Applications for Inverse **Design**: Sean Donegan¹; Edwin Schwalbach¹; Matthew Krug¹; ¹Air Force Research Laboratory

2:30 PM

High-throughput Alloy Design via Additive Manufacturing: Olivia Dippo¹; Kevin Kaufmann¹; Grant Schrader¹; Kenneth Vecchio¹; ¹University of California San Diego

2:50 PM

Alloy Design for Additive Manufacturing: Mariam Assi¹; Julien Favre¹; Anna Fraczkiewicz¹; Franck Tancret²; ¹Mines Saint-Etienne, Univ Lyon, LGF - UMR 5307 CNRS/ Centre SMS; ²Université de Nantes, Institut des Matériaux Jean Rouxel (IMN), Polytech Nantes, BP 50609

3:10 PM Invited Multi-objective Lattice Optimization Using an Efficient Neural Network Approach: Anthony Garland¹; Ben White¹; Brad Boyce¹; Ryan Alberdi¹; ¹Sandia National Labs

3:40 PM

Design of Ti-Al-Cr-V Alloys for Maximum Thermodynamic Stability: Rajesh Jha; George Dulikravich¹; ¹Florida International University



Prediction of the Mechanical Properties of Aluminum Alloy Using Bayesian Learning for Neural Networks: Shimpei Takemoto¹; Kenji Nagata²; Takeshi Kaneshita¹; Yoshishige Okuno¹; Katsuki Okuno¹; Masamichi Kitano¹; Junya Inoue³; Manabu Enoki³; ¹Showa Denko K.K.; ²National Institute for Materials Science; ³The University of Tokyo

4:20 PM

Machine Learning Assisted Exploration of FeCoCrNi Based Nanocrystalamorphous Dual-phase Alloys: Yi Yao¹; Xiaobing Hu²; Xiaoxiang Yu²; Jiaqi Gong¹; Feng Yan¹; Lin Li¹; ¹The University of Alabama; ²Northwestern University

4:40 PM

Topology Optimization for Design of Stress-dependent Material Properties: Justin Unger¹; Matthew Vaughn¹; Andrew Gaynor²; Brandon McWilliams²; James Guest¹; Kevin Hemker¹; ¹Johns Hopkins University; ²CCDC U.S. Army Research Laboratory

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering -**Computational Models and Algorithms in Atomistic Scale**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail



Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Tuesday PM March 16, 2021

Session Chair: Ebrahim Asadi, University of Memphis

2:00 PM

Characterizing Atomistic Geometries and Potential Functions Using Strain **Functionals**: *Edward Kober*¹; Colin Adams¹; Jacob Tavenner²; Nithin Mathew¹; ¹Los Alamos National Laboratory; ²Colorado School of Mines

2:20 PM

Modeling Static Recrystallization within the SPParKS Kinetic Monte Carlo Framework for Polycrystalline Materials: Austin Gerlt¹; David Newell²; Adam Pilchak²; Eric Payton²; ¹The Ohio State University; ²Air Force Research Lab

2:40 PM Invited

Characterizing the Length Dependence of High-Peierls-Stress Dislocations' Mobility in BCC Crystals under Deformation at Finite Temperature from the Atomistic to the Mesoscale: Liming Xiong¹; ¹Iowa State University

3:10 PM

Dislocation Dipole Study on Material Hardening/Softening: Abu Siddique¹; Tariq Khraishi¹; Hojun Lim²; ¹University of New Mexico; ²Sandia National Laboratories

3:30 PM

Continuum Dislocation Dynamics with Junction Reactions: Computational Modeling and Preliminary Results: Kyle Starkey¹; Anter El-Azab¹; ¹Purdue University



2:00 PM Invited

3:50 PM

Advancements in Discrete Dislocation Modeling of Slip Transmission through Equilibrium and Non-equilibrium Grain Boundaries: Darshan Bamney¹; Laurent Capolungo²; Douglas Spearot¹; ¹University of Florida; ²Los Alamos National Laboratory

ELECTRONIC MATERIALS

Alloys and Compounds for Thermoelectric and Solar Cell Applications IX — Session IV

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Hsin-Jay Wu, National Chiao Tung University; Sinn-wen Chen, National Tsing Hua University; Franck Gascoin, Cnrs Crismat Unicaen; Philippe Jund, Montpellier University; Yoshisato Kimura, Tokyo Institute of Technology; Lan Li, Boise State University; Takao Mori, National Institute for Materials Science; Tiejun Zhu, Zhejiang University; Alexandra Zevalkink, Michigan State University; Wan-Ting Chiu, Tokyo Institute of Technology

Tuesday PM March 16, 2021

Session Chairs: Wan-Ting Chiu, Tokyo Institute of Technology; Ping-Yuan Deng, National Chiao Tung University



TUESDAY PM

TABLE

Q

MOBILE-FRIEND

Structure and Physical Properties of Complex Chalcogenides: Fundamental Research with an "Eye" Towards Lower Temperature Applications: George Nolas¹; ¹University of South Florida

2:20 PM

Phase Boundary Mapping to Improve Na solubility, Band Convergence, and Thermoelectric Properties in p-type PbTe: *James Male*¹; Priyanka Jood²; Shashwat Anand¹; G. Snyder¹; ¹Northwestern University; ²National Institute of Advanced Industrial Science and Technology

2:40 PM

Defect Evolution Enabling Low Thermal Conductivity and High Thermoelectric Performance for n-type PbTe

: *Ping-Yuan Deng*¹; Kuang-Kuo Wang²; Jia-Yu Du³; Hsin-Jay Wu¹; ¹National Chiao Tung University; ²National Sun Yat-sen University; ³National Tsing Hua University

3:00 PM Invited

Thermal and Electrical Transport in Zintl Thermoelectrics: From Ab Initio Understanding to Materials Discovery: *Geoffroy Hautier*¹; ¹Université catholique de Louvain

3:20 PM Invited The "Grand Challenge" of Thermoelectric Materials: *David Parker*¹; ¹ORNL

3:40 PM Invited The Origin of Low Thermal Conductivity in Tetrahedrites: A Jahn-Teller Electronic Instability: *Paz Vaqueiro*¹; ¹University of Reading

4:00 PM Invited

Effect of Phonon Drag on Seebeck Coefficient Based on Linear Response Theory: Masao Ogata¹; Junya Endo¹; Hiroyasu Matsuura¹; Hideaki Maebashi¹; Hidetoshi

Fukuyama²; ¹University of Tokyo; ²Tokyo University of Science

2:00 PM The Effect of Rare Earth Mischmetal on the High Temperature Tensile Properties of

4:20 PM Invited

Strategies for the Balance of Oxide/Metal Composites Towards the Applications of Flexible Solar Energy Harvesters: Wan-Ting Chiu¹; Chang Tso-Fu Mark¹; Masato Sone¹; Agnes TIXIER-MITA²; Hiroshi Toshiyoshi²; Hideki Hosoda¹; ¹Tokyo Institute of Technology; ²The University of Tokyo

4:40 PM

Effect of Zn and Cr Co-doping on the Thermoelectric Properties of Colusite Cu26V2M6S32 (M=Ge,Sn): Paulina Kaminska¹; Cédric Bourgès²; Piotr Spiewak¹; Takao Mori²; ¹Warsaw University of Technology; ²National Institute for Materials Science

LIGHT METALS

Aluminum Alloys, Processing and Characterization — Mechanical Properties, **Applications, and Fitness for Service Testing**

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Dimitry Sediako, University of British Columbia

Tuesday PM March 16, 2021

Session Chair: Nima Shamsaei, Auburn University

ONTENTS FABLE Q





TUESDAY PM

an A356 Aluminum Alloy: Joshua Stroh¹; Dimitry Sediako¹; David Weiss²; ¹University of British Columbia Okanagan; ²Eck Industries

2:20 PM

Effects of Ultrasonic Melt Processing on Microstructure, Mechanical Properties and Electrical Conductivity of Hypereutectic Al-Si, Al-Fe and Al-Ni Alloys with Zr Additions: Suwaree Chankitmunkong¹; Dmitry Eskin²; Chaowalit limmaneevichitr¹; ¹King Mongkut's University of Technology Thonburi; ²Brunel University London

2:40 PM

The Corrosion Behavior of 5xxx and 6xxx Aluminum Alloys with Trace Calcium: Saugat Singh¹; Kumar Sundaram²; B. Pesic¹; ¹University of Idaho; ²Novelis Molten Metal Processing, Novelis Corporation

3:00 PM

Review of Retrogression Forming and Reaging for AA7075-T6 Sheet: Katherine *Rader*¹; Jon Carter²; Louis Hector²; Eric Taleff¹; ¹University of Texas at Austin; ²General Motors

3:20 PM

Fatigue and Failure Analysis of an Additively Manufactured Contemporary Aluminum Alloy: P.D. Nezhadfar¹; Spencer Thompson²; Ankit Saharan²; Nam Phan³; Nima Shamsaei¹; ¹Auburn University; ²EOS North America; ³Structures Division, Naval Air Systems Command (NAVAIR)

3:40 PM

Investigation of Weld Quality for Friction Stir Welding of Extrued 6XXX Series Aluminium Alloys: Mehmet Bugra Guner¹; *Murat Konar*; Arif Fatih Yigit¹; Görkem Özçelik¹; Tolga Demirkiran¹; ¹Asas Aluminium

4:00 PM

The Effect of Al3Er Particles on the Structure and Mechanical Properties of an Al-Mg Alloy: Anton Khrustalev¹; Ilya Zhukov¹; Vladimir Platov¹; Alexander Vorozhtsov¹;

¹Tomsk State University

4:20 PM Question and Answer Period

LIGHT METALS

Aluminum Reduction Technology Across the Decades: An LMD Symposium Honoring Alton T. Tabereaux and Harald A. Øye – Alton Tabereaux Honorary Session: Reduction Cell Operation and Process Control - Joint session with **Aluminum Reduction Technology**

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Arne Ratvik, SINTEF; Marc Dupuis, GeniSim Inc.; Kristian Etienne Einarsrud, Norwegian University of Science and Technology

Tuesday PM March 16, 2021

Session Chair: Marc Dupuis, GeniSim Inc.

2:00 PM

Introductory Comments: Aluminum Reduction Technology Across the Decades: An LMD Symposium Honoring Alton T. Tabereaux and Harald A. Øye: Marc Dupuis¹; ¹GeniSim Inc.

2:05 PM

Alton Tabereaux: A Humble Individual Who Dedicates His Lifetime to Aluminum



- An Aluminum Legend of Our Time: Xiangwen Wang¹; ¹Alcoa Corp

2:45 PM

Awakening of the Aluminum Industry to PFC Emissions and Global Warming: *Alton Tabereaux*¹; David Wong¹; ¹Consultant

3:05 PM

Application and Adapta bility of MHD Stability Computation for Modern Aluminium **Reduction Cells at Extreme Conditions of Low ACD**: Valdis Bojarevics¹; *Marc Dupuis*²; ¹University of Greenwich; ²GeniSim Inc.

3:25 PM

Investigation of Cyclic Process Variations within Hall-Héroult Reduction Cells: Jayson Tessier¹; Samuel Duplessis¹; ¹Alcoa

3:45 PM

In Line Cell Position and Anode Change Effects on the Alumina Dissolution: Valdis *Bojarevics*¹; ¹University of Greenwich

4:05 PM

History of Computer Control of Aluminum Reduction Cells: Vinko Potocnik¹; Michel Reverdy¹; ¹Vinko Potocnik Consulting

4:25 PM Question and Answer Period

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII — Alloy Development and Application II



Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa **Technical Center**

March 16, 2021 **Tuesday PM**

Session Chairs: Eun Park, Seoul National University; David Browne, University College Dublin

2:00 PM

Fabrication of Fe-based Metallic Glassy Microparts Through Unprecedented **Processes**: *Rui Yamada*¹; Noriharu Yodoshi¹; Naoyuki Nomura¹; Junji Saida¹; Akira Kawasaki¹; ¹Tohoku University

2:20 PM Invited

Selection and Testing of Bulk Metallic Glass Alloys for Space-based Mechanisms: Andrew Murphy¹; Andrew Norman²; David Browne¹; ¹University College Dublin; ²European Space Agency

2:45 PM

Measuring Metallic Glass Viscosities Over Wide Composition Ranges: Sebastian *Kube*¹; Theo Evers¹; Will Polsky¹; Rodrigo Miguel Ojeda Mota¹; Kevin Ryan¹; Jan Schroers¹; ¹Yale University

MOBILE-FRIENDL

3:05 PM

Machine Learning from Elemental and Simulation Features for Predicting Glass Forming Ability: Dane Morgan¹; Benjamin Afflerbach¹; Lane Schultz¹; Janine Erickson¹; Dan Thoma¹; John Perepezko¹; Carter Francis¹; Paul Voyles¹; George Bokas²; Jianqi Xi¹; Izabela Szlufarska¹; ¹University of Wisconsin-Madison; ²Siemens **Industry Software**

LIGHT METALS

Cast Shop Technology — Recycling and Furnace Operations

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Samuel Wagstaff, Oculatus

Tuesday PM March 16, 2021

Session Chairs: Kjerstin Ellingsen, SINTEF; Jean-Francois Desmeules, Dynamic Concept

2:00 PM Introductory Comments: Cast Shop Technology: Samuel Wagstaff¹; ¹Oculatus

2:05 PM Impact of COVID-19 on the British Foundries: Prateek Saxena¹; Pam Murrell²; Tharmalingam Sivarupan³; Konstantinos Salonitis¹; Mark Jolly¹; ¹Cranfield University; ²Cast Metals Federation; ³The University of Queensland



2:25 PM

Effect of Steam on Aluminium Packaging Multilayers: Martin Syvertsen¹; Anne Kvithyld¹; Birgitte Vågenes¹; Stephan Kubowicz¹; Rune Gaarder¹; ¹SINTEF Industry

2:45 PM

Compaction of Aluminium Foil and Its Effect on Oxidation and Recycling Yield: Alicia Vallejo Olivares¹; Harald Philipson¹; Mertol Gökelma²; Hans Roven¹; Trond Furu³; Anne Kvithyld⁴; Gabriella Tranell¹; ¹Norwegian University of Science and Technology; ²Izmir Institute of Technology; ³Norsk Hydro; ⁴SINTEF

3:05 PM

Influence of Mg Concentration on the Inhibiting Effect of CO, on the Oxidation Rate of Aluminum Alloys 5182 and 6016: *Cathrine Solem*¹; Egil Solberg²; Gabriella Tranell¹; Ragnhild Aune¹; ¹Norwegian University of Science and Technology (NTNU); ²Alcoa Norway ANS

3:25 PM

Automated Chemical Analysis of Liquid Aluminum for Process Control: Sveinn Hinrik Gudmundsson¹; Halldor Gudmundsson²; *Kristjan Leosson*¹; ¹DT Equipment; ²Nordural ehf.

3:45 PM

Characteristic Impurities of Silicon Metal SI-441 as Additive Material to Produce Aluminium Foundry Alloy A356.2: Reggy Zurcher¹; Rainaldy Harahap¹; Edi Mugiono¹; M. Yasir Parapat¹; Masrul Ponirin¹; ¹PT Indonesia Asahan Aluminium

4:25 PM Question and Answer Period

ONTENTS

FABLE OF



TUESDAY PM

Molten Aluminium Transfer: Review and Comparison of Different Technologies: *Olivier Dion-Martin*¹; Robert Dumont¹; Jean Francois Desmeules¹; ¹Dynamic Concept

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Characterization of **Composite Materials**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

March 16, 2021 **Tuesday PM**

Session Chairs: Sergio Monteiro, Military Institute of Engineering; Kelvin Xie, Texas A&M University

2:00 PM

Composite Binder and Particle Size Effects on Mechanical Properties of Nonhazardous High Explosive Surrogates: Matthew Herman¹; Caitlin Woznick¹; Amanda Duque¹; John Yeager¹; ¹Los Alamos National Laboratory



4:00 PM

2:20 PM

Mechanical Testing and Microstructural Investigation into the Effects of Heat Treatment on Additively Manufactured TiC Reinforced Ti-Ni Matrix Composites (TNMCs): Andrew Dodd¹; Jianshen Wang¹; Daniel East²; Evgeny Morozov¹; Juan Escobedo-Diaz¹; ¹University of New South Wales; ²CSIRO Manufacturing

2:40 PM

Influence of Graphene Oxide Fuctionalization Strategy on the Dynamic Mechanical Response of Natural Fiber Reinforced Polymer Matrix Composites: *Fabio Garcia Filho*¹; Michelle Oliveira¹; Fernanda Luz¹; Sergio Monteiro¹; ¹Military Institute of Engineering

3:00 PM

Charpy Impact Tests of Castor Oil Derived Polyurethane Matrix Composites Reinforced by Wood Industry Waste: Juliana de Faria¹; Noan Simonassi¹; Carlos Maurício Vieira¹; *Felipe Lopes*²; ¹State University of Northern Rio de Janeiro; ²UENF

3:20 PM

FlexuralStrengthofCastorOilDerivedPolyurethaneMatrixCompositeReinforced with Luffa Fibers: Anna Carolina Cerqueira Neves¹; Noan Simonassi²; *Felipe Lopes*¹; Carlos Mauricio Vieira¹; ¹UENF; ²State University of Northern Rio de Janeiro

3:40 PM

Spall Damage Characterization of Additively Manufactured Ti-Ni-C Composites: Warwick Absolon¹; Jianshen Wang¹; Daniel East²; Ali Ameri¹; Hongxu Wang¹; Evgeny Morozov¹; Paul Hazell¹; *Juan Escobedo-Diaz*¹; ¹University of New South Wales; ²CSIRO Manufaturing





Characterization of Equimolar Zinc Ferrite - ZF: *Mery Gomez-Marroquin*¹; José Carlos D'Abreu²; Henry Colorado³; Abraham Terrones - Ramírez⁴; Kim Phatti - Satto⁴; Nilton Cárdenas-Falcón⁵; ¹APMMM/UNI; ²DEQM PUC-Rio; ³University of Antioquia - UDEA; ⁴FIGMM UNI; ⁵PUCP

4:20 PM

Characterization of Ultra-hard Ceramic AlMgB14-based Materials Obtained by Self-propagating High-temperature Synthesis and Spark Plasma Sintering: Ilya Zhukov¹; *Pavel Nikitin*¹; Alexander Vorozhtsov¹; ¹Tomsk State University

4:40 PM

Preparation of Ceramic Coating on Copper Substrate with Transitional Layer by Low-temperature Slurry Method: *Zefei Zhang*¹; Hao Bai¹; Lihong Li²; Min Zhong²; ¹University of Science and Technology Beijing; ²Shantou Huaxing Metallurgical Equipment Co., Ltd.

NUCLEAR MATERIALS

Characterization of Nuclear Materials and Fuels with Advanced X-ray and Neutron Techniques — X-ray Tomography and Microscopy

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Nuclear Materials Committee

Program Organizers: Xuan Zhang, Argonne National Laboratory; Jonathan Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University; Joshua Kane, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory; J. Kennedy, Idaho National Laboratory; Arthur Motta, Pennsylvania State University

TMS





Session Chairs: Joshua Kane, Idaho National Laboratory; Xuan Zhang, Argonne National Laboratory

2:00 PM

Characterization of Nuclear Energy Materials in 2D and 3D using Laboratorybased X-ray Microscopy: *Nikolaus Cordes*¹; Joshua Kane¹; Aaron Craft¹; ¹Idaho National Laboratory

2:20 PM

Non-destructive Correlative 3D Characterization of Nuclear Graphite: From the Microscale to the Nanoscale: Stephen Kelly¹; *Robin White*¹; William Harris¹; Tobias Volkenandt¹; Benjamin Tordoff¹; Giuliano Laudone²; Katie Jones²; Ben Veater²; ¹Carl Zeiss X-ray Microscopy; ²University of Plymouth

2:40 PM

Irradiation Effects on Precipitate Distributions in High-temperature Ultrafineprecipitate-strengthened Steel Characterized by Synchrotron Micro-computed Tomography: *Alejandro Figueroa*¹; Sri Nori¹; Peter Kenesei²; Jonathan Almer²; Maria Okuniewski¹; ¹Purdue University; ²Argonne National Laboratory

3:00 PM

Identifying the Microstructural Origins of Creep Damage in Alloy 617: Mark Messner¹; Xuan Zhang¹; Meimei Li¹; Michael McMurtrey²; ¹Argonne National Laboratory; ²Idaho National Laboratory

3:20 PM

Getting "Around" the High Mass Attenuation Issue for µX-ray Computed



Tomography of Nuclear Fuels: *Joshua Kane*¹; Nikolaus Cordes¹; Aaron Craft¹; Douglas Marshall¹; John Stempien¹; ¹Idaho National Laboratory

NUCLEAR MATERIALS

Composite Materials for Nuclear Applications — Composite Fuels/Graphite Carbon

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee, TMS: Nuclear Materials Committee

Program Organizers: Anne Campbell, Oak Ridge National Laboratory; Dong Liu, University of Bristol; Rick Ubic, Boise State University; Lauren Garrison, Oak Ridge National Laboratory; Peng Xu, Idaho National Laboratory; Johann (Hans) Riesch, Max Planck Institute for Plasma Physics

Tuesday PM March 16, 2021

Session Chair: Anne Campbell, Oak Ridge National Laboratory

2:00 PM Invited

Improved Techniques for Determining Local Thermal Transport in Composite Nuclear Fuels: Scott Middlemas¹; Joshua Kane¹; Tsvetoslav Pavlov¹; Boopathy Kombaiah¹; Daniel LaBrier²; Yu-lin Shen³; Isabella Van Rooyen¹; ¹Idaho National Laboratory; ²Idaho State University; ³University of New Mexico

2:30 PM Invited

Overview of the Westinghouse Accident Tolerant and High Burnup Fuel Program: *Edward Lahoda*¹; Zeses Karoutas¹; Luke Olson¹; Luther Hallman¹; Kathryn Metzger¹;

Jorie Walters¹; Michael Sivack¹; John Lyons¹; Luke Czerniak¹; Allan Jaworski¹; Ben Maier¹; Robert Terry¹; Zachary McDaniel¹; Frank Boylan¹; Jeffrey Kobelak¹;

Michael Shockling¹; Magnus Limback¹; Antoine Claisse¹; Jonathan Wright¹; John Ghergurovich¹; ¹Westinghouse Electric

3:00 PM

Development of UN/UO2 Composite Fuels for LWR Applications: *Peng Xu*¹; Lingfeng He¹; Brian Jaques²; Kumar Sridharan³; Darryl Butt⁴; ¹Idaho National Laboratory; ²Boise State University; ³University of Wisconsin; ⁴University of Utah

3:20 PM

Uranium Nitride Advanced Fuel: An Evaluation of the Oxidation Resistance of **Coated and Doped Grains**: *Yulia Mishchenko*¹; Denise Adorno Lopes²; Kyle Johnson³; Janne Wallenius¹; ¹KTH; ²Westinghouse Electric Company; ³Studsvik Nuclear AB

3:40 PM

Fabrication. Characterisation and Oxidation Resistance of an Innovative Composite Fuel: UN Microspheres Embedded in UO, Matrix: Diogo Costa¹; Marcus Hedberg²; Simon Middleburgh³; Janne Wallenius⁴; Pär Olsson⁴; Denise Lopes⁵; ¹KTH Royal Institute of Technology, Westinghouse Electric Sweden AB; ²Chalmers University of Technology; ³Bangor University; ⁴KTH Royal Institute of Technology; ⁵Westinghouse Electric Sweden AB

4:00 PM Invited

Use of Carbon Fibre-reinforced Carbon in Wendelstein 7-X: Jean Boscary¹; Henri Greuner¹; Boris Mendelevitch¹; Gunnar Ehrke¹; Patrick Junghanns¹; Reinhold Stadler¹; ¹Max-Planck-Institut für Plasmaphysik

4:30 PM

Sub-critical Crack Initiation, Coalescence and Propagation in Nuclear Graphite Studied by High-speed Pink Beam Synchrotron Tomography: Thomas Zillhardt¹;



TUESDAY PM

TABLE OF

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics — Phase Stability I

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

Tuesday PM March 16, 2021

Session Chairs: Mira Todorova, Max Planck Institut fur Eisenforschung; Jorge Munoz, University of Texas El Paso; Hong Liu, KU Leuven; Eva Zarkadoula, Oak Ridge National Laboratory

2:00 PM Invited

Integrated Models for the Design of Precipitation Hardenable Mg and Al Alloys: Hong Liu¹; Ioannis Papadimitriou²; Fengxiang Lin³; Javier Llorca⁴; Jian-Feng Nie⁵; Moelans Nele¹; ¹KU Leuven; ²IMDEA Materials ; ³UC Louvain ; ⁴IMDEA Materials; ⁵Monash University

2:30 PM

Competing and Collaborating Phase Transitions Studied within Cluster Variation

Method: *Tetsuo Mohri*¹; ¹Tohoku University

VEBSITE TMS

First principles Study of Precipitation in Al-Cu, Al-Li and Al-Cu-Li Alloys: Sha Liu¹; Javier Llorca²; ¹IMDEA Materials Institute; ²IMDEA Materials Institute & Technical University of Madrid

3:10 PM Invited Insights into Processes at Electrochemical Solid/Liquid Interfaces from Ab Initio Molecular Dynamics Simulations: Mira Todorova¹; Sudarsan Surendralal¹; Stefan Wippermann¹; Florian Deissenbeck¹; Christoph Freysoldt¹; Joerg Neugebauer¹; ¹Max Planck Institut fur Eisenforschung

3:40 PM

2:50 PM

Effect of Oxygen on Joining Magnesium and Iron: Insights from Ab Initio Simulations: Peter Sushko¹; Yingge Du¹; Hrishikesh Das¹; Piyush Upadhyay¹; ¹Pacific Northwest National Laboratory

4:00 PM

A First-principles Analysis of the Temperature Dependence of Stacking Fault Energies in Mg and Ti: Julian Brodie¹; Maryam Ghazisaeidi¹; ¹Ohio State University

4:20 PM Invited

Vacancy-mediated Phase Selection in High-entropy Alloys: Prashant Singh¹; Shalabh Gupta¹; A V Smirnov¹; Matthew J Kramer¹; Duane D Johnson¹; ¹Ames Laboratory

4:50 PM

Lattice Dynamics of FeTi at Simultaneous High Temperature and High Pressure from First Principles: Adrian De la Rocha¹; *Jorge Munoz*¹; Armando Garcia¹; Vanessa Meraz¹; Bethuel Khamala¹; Bert de Jong²; Yu-Hang Tang²; ¹The University of Texas



TUESDAY PM TABLE OF

PHYSICAL METALLURGY

Defect and Phase Transformation Pathway Engineering for Desired Microstructures — Simulation and Modeling

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Yufeng Zheng, University of Nevada-Reno; Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Timofey Frolov, Lawrence Livermore National Laboratory; Stoichko Antonov, Max-Planck-Institut für Eisenforschung GmbH; Jessica Krogstad, University of Illinois at Urbana-Champaign; Bin Li, University of Nevada, Reno

March 16, 2021 **Tuesday PM**

Session Chair: Yipeng Gao, Idaho National Laboratory

2:00 PM

Interactions between Lattice Dislocations and 3D Metallic Interfaces: Shuozhi *Xu*¹; Justin Cheng²; Nathan Mara²; Irene Beyerlein¹; ¹University of California, Santa Barbara; ²University of Minnesota, Twin Cities

2:20 PM

Interfacial Segregation and Segregation-induced Transitions in a Polycrystalline Grain Boundary Network: *Pulkit Garg*¹; Zhiliang Pang²; Vladyslav Turlo³; Timothy Rupert⁴; ¹Arizona State University; ²Guilin University of Electronic Technology;

³Swiss Federal Laboratories for Materials Science and Technology (Empa); TMS WEBSITE

⁴University of California, Irvine

2:40 PM Twin Boundaries Continue to Surprise Us: Understanding Type II Twin in NiTi and [1012] Twin in HCP Materials: *Ahmedsameerkhan Mohammed*¹; Huseyin Sehitoglu¹; ¹University of Illinois Urbana-Champaign

3:00 PM

New Insights into The Effect of Solutes on Twinning in Ti Alloys: *Mohammad Shahriar Hooshmand*¹; Yan Chong¹; Ruopeng Zhang¹; Andrew Minor¹; Mark Asta¹; ¹University of California, Berkeley

3:20 PM

Evolving Core Structures in Dislocation-twin Boundary Interactions: Orcun Koray Celebi¹; Ahmed Sameer Khan Mohammed¹; Francisco Andrade Chávez¹; Jessica Krogstad¹; Huseyin Sehitoglu¹; ¹University of Illinois Urbana Champaign

3:40 PM

Characterizing and Modeling Collective Atomic Displacements during Grain Boundary Migration: *Ian Chesser*¹; Anqi Qiu¹; Ankit Gupta²; Garritt Tucker²; Brandon Runnels³; Elizabeth Holm¹; ¹Carnegie Mellon University; ²Colorado School of Mines; ³University of Colorado Colorado Springs

4:00 PM

Assessment and Design of Complex Microstructural Features in Zirconia Shape Memory Ceramics via Elasto-Plastic Phase-field Modeling: *Cheikh Cissé*¹; Mohsen Asle Zaeem¹; ¹Colorado School of Mines

4:20 PM

Pseudoelastic Response of Ion-implanted Nickel-titanium Shape Memory Alloy:



Combining Experimentation and Forward Modeling: *Daniel Hong*¹; Harshad Paranjape²; Peter Anderson¹; Alejandro Hinojos¹; Michael Mills¹; Khalid Hattar³; Nan Li⁴; Jeremy Schaffer⁵; ¹The Ohio State University; ²Confluent Medical; ³CINT Sandia National Laboratories; ⁴CINT Los Alamos National Laboratories; ⁵Fort Wayne Metals

4:40 PM

Investigation of Nucleation Mechanisms Associated with Formation of Coprecipitates in Ni-based Superalloys: *Hariharan Sriram*¹; Semanti Mukhopadhyay¹; Rongpei Shi²; Michael Mills¹; Yunzhi Wang¹; ¹The Ohio State University; ²Lawrence Livermore National Laboratory

MATERIALS PROCESSING

Deformation Induced Microstructural Modification — Session IV: Deformation of Alloys I

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside ; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

Tuesday PM March 16, 2021

Session Chair: Daniel Coughlin, Los Alamos National Laboratory

2:00 PM Invited Deformation Induced Precipitation (DIP) in Light Alloys: Theory and Experiments: Suhas Eswarappa Prameela¹; Peng Yi¹; Yannick Hollenweger²; Laszlo Kecskes¹;

Dennis Kochmann²; Michael Falk¹; *Timothy Weihs*¹; ¹Johns Hopkins University; ²ETH Zurich

2:30 PM

Cyclic Deformation and Fatigue Behavior of 316L Stainless Steel Processed by Surface Mechanical Rolling Treatment: *Luiz Carneiro*¹; Xiaogui Wang²; Yanyao Jiang¹; ¹University of Nevada, Reno; ²Zhejiang University of Technology

2:50 PM

HighPressureTorsionProcessedMaragingSteels:MicrostructureandMechanical Behaviour: *Kevin Jacob*¹; Deepesh Yadav¹; Saurabh Dixit²; Anton Hohenwarter³; Balila Jaya¹; ¹IIT Bombay; ²Mishra Dhatu Nigam Ltd.(Midhani); ³Montanuniversität Leoben

3:10 PM Invited

Fabrication of Ultrafine Grained Ferritic Steels by Combining Dynamic Transformation and Dynamic Recrystallization: *Nobuhiro Tsuji*¹; Lijia Zhao²; Nokeun Park³; Yanzhong Tian⁴; Akinobu Shibata⁵; ¹Kyoto University; ²ArcelorMittal; ³Yeungnam University; ⁴Northeastern University; ⁵National Institute for Materials Science

3:40 PM Invited

Microstructural Evolution and Deformation Mechanisms in Segregation-Engineered Nanocrystalline Al Alloys: Glenn Balbus¹; Johann Kappacher²; David Sprouster³; Jungho Shin⁴; Fulin Wang⁴; Jason Trelewicz³; Daniel Kiener²; Verena Maier-Kiener²; *Daniel Gianola*⁴; ¹UCSB; ²Montanuniversität Leoben; ³Stony Brook University; ⁴University of California, Santa Barbara **MOBILE-FRIEND**



The Effect of Processing Parameters on the Microstructure and Performance of Ni-Mn-Ga Alloys: *Pnina Ari-Gur*¹; Pranav Bhale¹; Irek Musabirov²; Ronald Noebe³; Vladimir Shavrov⁴; Victor Koledov⁴; ¹Western Michigan University; ²Russian Academy of Sciences, Ufa; ³NASA Glenn Research Center; ⁴Russian Academy of Sciences, Moscow

4:30 PM

Thermomechanical Processing of Dilute Mg-Zn-Ca Alloys: *Jenna Krynicki*¹; Laszlo Kecskes¹; John Gibbins¹; Zhigang Xu²; Timothy Weihs¹; ¹Johns Hopkins University; ²North Carolina A&T State University

ELECTRONIC MATERIALS

Electronic Packaging and Interconnections 2021 — Pb-free Solder Alloys II

Sponsored by: TMS Functional Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Mehran Maalekian, Mat-Tech; Christopher Gourlay, Imperial College London; Babak Arfaei, Ford Motor Company; Praveen Kumar, Indian Institute of Science; Sai Vadlamani, Intel Corporation; Kazuhiro Nogita, University of Queensland; David Yan, San Jose State University

Tuesday PM March 16, 2021

Session Chairs: Christopher Gourlay, Imperial College London; David Yan, San José State University

2:00 PM Invited Effect of Current Stress on the Microstructure of SnBiAg-SAC Mixed Solder Joints: *Eric Cotts*¹; Faramarz Hadian¹; Randy Owen¹; ¹Binghamton University

- , .

CORROSION

2:20 PM Effects of Antimony on the Microstructure and Reliability of Sn-Ag-Cu-based **Solder Joints**: Sergey Belyakov¹; Richard Coyle²; Babak Arfaei³; *Christopher Gourlay*¹; ¹Imperial College London; ²Nokia Bell Laboratories; ³Ford Motor Company

2:40 PM Invited Sn-Ag-Cu and Sn-Bi Solder Powders for Fine Pitch Printing: Amir Nobari¹; Arslane Bouchemit²; Gilles L'Espérance²; ¹5N Plus Inc - Micro Powders; ²École Polytechnique de Montréal

3:00 PM Invited Single Solder Joint Shear with In-situ Current Stressing: Kendra Young¹; Choong-Un Kim²; *Tae-Kyu Lee*¹; ¹Portland State University; ²University of Texas, Arlington

3:20 PM

Solderability Assessment of Lead-free Alloys: Mehran Maalekian¹; ¹Mat-Tech

3:40 PM

Finite Element Analysis Modeling of Stress Evolution and Whisker Growth Under Applied Pressure: Nupur Jain¹; Piyush Jagtap¹; Allan Bower¹; Eric Chason¹; ¹Brown University

4:00 PM

Corrosion Behavior of Co-based Surface Finishes in Sulfur-containing Gas: Si-Wei Lin¹; Albert T. Wu¹; ¹National Central University

TABLE

Q

NTENTS





Environmentally Assisted Cracking: Theory and Practice – Stress Corrosion Cracking I

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Tuesday PM March 16, 2021

Session Chairs: Karl Sieradzki, Arizona State University; Yong Yang, University of Florida

2:00 PM

Finite Element Modeling and Uncertainty Quantification of Stressed Corrosion Behavior in Aluminum Alloys: Kaiwen Wang¹; Yinan Wang¹; Xiaowei Yue¹; Wenjun Cai¹; ¹Virginia Polytechnic Institute and State University

2:20 PM

Understanding the Effects of B-phase Precipitation on the Stress Corrosion Cracking Performance of Thin Plate 5xxx Alloys: William Golumbfskie¹; Matthew McMahon¹; Emily Holcombe¹; Mitra Taheri²; ¹Naval Surface Warfare Center, Carderock Division; ²Johns Hopkins University

2:40 PM Invited Stress Corrosion Cracking Behavior of the Addictively Manufactured 316L **Stainless Steel**: Yong Yang¹; ¹University of Florida



3:20 PM

SCC Performance of Repaired 304L: *Gabriella Marino*¹; J. Srinivasan¹; B. Sutton¹; J. Li¹; G. Daehn¹; A. Vivek¹; R. Thodla²; A. Shapiro³; A. Ramirez¹; J. Locke¹; ¹The Ohio State University; ²DNV GL; ³The Ohio State University, Titanium Brazing Inc.

3:40 PM

Irradiation-assisted Stress Corrosion Cracking (IASCC) of Austenitic Stainless Steels with Oversized Solutes in High-temperature Water: *Jingfan Yang*¹; Xiang Liu²; Miao Song³; Lingfeng He²; Yongfeng Zhang⁴; Xiaoyuan Lou¹; ¹Auburn University; ²Idaho National Laboratory; ³University of Michigan; ⁴University of Wisconsin

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and Computational Modeling — Advanced Experimental Characterization of Microstructurally Driven Fatigue Behavior

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear, University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara



TUESDAY PM

TABLE

Q

ONTENTS

Tuesday PM March 16, 2021

Session Chair: Garrett Pataky, Clemson University

2:00 PM Invited Microstructure and Fatigue Damage Evolution in Additive-manufactured Metals Using Enhanced Measurement Techniques and Modeling Approaches: *Mustafa Awd*¹; Frank Walther¹; Ali Fatemi²; ¹TU Dortmund University; ²University of Memphis

2:20 PM

Low Cycle Fatigue Behavior of an Optimally Produced

Additive Manufactured Aluminum Alloy: *Emine Tekerek*¹; Vignesh Perumal¹; Darren Beckett²; Scott Halliday³; Antonios Kontsos¹; ¹Drexel University; ²Sigma Labs; ³Navajo Technical University

2:40 PM

Investigation of the Fatigue Crack Behavior of 304 Stainless Steels Using Synchrotron X-ray Tomography: *Ryan Schoell*¹; Li Xi¹; Harvey West¹; Zeev Shayer²; Djamel Kaoumi¹; ¹North Carolina State University; ²Colorado School of Mines

3:00 PM

Long Range Internal Stress Assessment Using Convergent Beam Electron Diffraction and Dislocation Dipole Height in Cyclically Deformed Copper Single Crystals: Roya Ermagan¹; Maxime Sauzay²; Michael Kassner¹; ¹University of Southern California; ²CEA Paris-Saclay

3:20 PM

Correlation between Cyclic Plastic Deformations and Strength Mismatches in Ni-Steel Dissimilar Joints under Isothermal Low-cycle Fatigue Tests: *Shutong*

TMS

Zhang¹; Sebastian Romo¹; Rafael Arthur Giorjao¹; Antonio Ramirez¹; ¹Ohio State



3:40 PM

High and Very High Cycle Fatigue Behavior of Additively Manufactured 17-4 PH Stainless Steel: The Effect of Shielding Gas: *P.D. Nezhadfar*¹; Jade Welsh²; Jutima Simsiriwong²; Shuai Shao¹; Nima Shamsaei¹; ¹Auburn University; ²University of North Florida

4:00 PM

An In-situ Analysis on the Fatigue Damage in Martensitic Spring Steel: *Anna Wildeis*¹; Matthias Thimm¹; Robert Brandt¹; Hans-Jürgen Christ¹; Claus-Peter Fritzen¹; ¹University of Siegen

4:20 PM

Post-fatigue Study of SLM Ti64 Medical Implant by 3D Correlative Microscopy: *Bartlomiej Winiarski*¹; Matteo Benedetti²; Philip Withers³; ¹Thermo Fisher Scientific; ²University of Trento; ³The University of Manchester

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Control & Non-Destructive Examination

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St.



Petersburg Polytechnic University

Tuesday PM March 16, 2021

2:00 PM

Real-time Measurement of Friction Stir Tool Motion during Defect Interaction in Aluminum Alloy 6061-T6: *Daniel Franke*¹; Frank Pfefferkorn¹; Shiva Rudraraju¹; Michael Zinn¹; ¹University of Wisconsin Madison

2:20 PM

Development of Automatic Quality Control Techniques for Friction Stir Welding Processes: *Egoitz Aldanondo*¹; ¹LORTEK

2:40 PM

Preliminary Investigation of the Effect of Temperature Control in Friction Stir Welding: *Johnathon Hunt*¹; David Pearl²; Carter Hamilton²; Yuri Hovanski¹; ¹Brigham Young University; ²Miami University

3:00 PM

Transitioning FSW to a Controlled Production Process: *Arnold Wright*¹; Devry Smith¹; Brandon Taysom²; Yuri Hovanski¹; ¹Brigham Young University; ²Pacific Northwest National Laboratory

3:20 PM

Removing Rotational Variations from Shoulder Thermocouples in Friction Stir Welding: *Brandon Taysom*¹; Kenneth Ross¹; Woongjo Choi¹; ¹Pacific Northwest National Laboratory

Frontiers in Solidification Science VIII — Faceted Growth / Solid-Liquid

Interfaces

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

March 16, 2021 **Tuesday PM**

Session Chairs: Mohsen Asle Zaeem, Colorado School of Mines; Damien Tourret, IMDEA Materials; Alain Karma, Northeastern University; Nana Ofori-Opoku, **Canadian Nuclear Laboratories**

2:00 PM Invited

3D Phase-field Simulations of Pattern Formation during Freeze Casting: Kaihua Ji¹; Kaiyang Yin¹; Louise Strutzenberg²; Rohit Trivedi³; Ulrike Wegst¹; *Alain Karma*¹; ¹Northeastern University; ²NASA Marshall Space Flight Center; ³Iowa State University

2:30 PM

Experimental Observations of Mechanisms of Pattern Formation during Freeze Casting: *Kaiyang Yin*¹; Kaihua Ji¹; Louise Strutzenberg²; Rohit Trivedi³; Alain Karma¹; Ulrike G.K. Wegst¹; ¹Northeastern University; ²NASA Marshall Space Flight Center;



2:50 PM Invited Combination of X-ray Topography and Radiography for In Situ and Time Resolved Investigation of the Solidification of Silicon: Hadjer Ouaddah¹; Gabrielle Regula¹; Guillaume Reinhart¹; *Nathalie Mangelinck-Noël*¹; ¹IM2NP CNRS UMR 7334, Aix Marseille University

3:20 PM

Facetted Growth in Isothermal Solidification of Silicon: 3D Phase-field Simulations of Growth and Equilibrium Shapes

: Ahmed Kaci Boukellal¹; Ahmed Kerim Sidi Elvalli²; Jean-Marc Debierre³; ¹Aix-Marseille University (IM2NP) and IMDEA Materials; ²Aix-Marseille University (IM2NP) and Spintec; ³Aix-Marseille University (IM2NP)

3:40 PM Invited

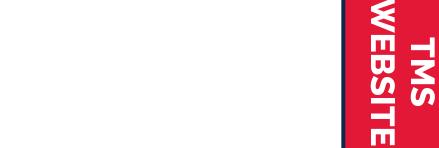
Bridging Multiscale Models for Predicting Nano and Microstructures in Rapid **Solidification of Metals and Alloys**: *Mohsen Asle Zaeem*¹; ¹Colorado School of Mines

4:10 PM

A Method of Estimation of Solid-liquid Interface Anisotropy Based on Machine Learning Combined with Phase-field Simulations: Geunwoo Kim¹; Tomohiro Takaki²; Yasushi Shibuta³; Munekazu Ohno¹; ¹Hokkaido University; ²Kyoto Institute of Technology; ³The University of Tokyo

4:30 PM

Structural Changes during Crystallization and Vitrification of Dilute FCC-based **Binary Alloys**: *Deep Choudhuri*¹; Bhaskar Majumdar¹; ¹New Mexico Institute of Mining and Technology



Unraveling the Effect of Solid-liquid Interfacial Anisotropy on Pattern Formation in Rapid Directional Solidification of Binary Alloys: *Ghavam Azizi*¹; Mohsen Asle Zaeem¹; ¹Colorado School of Mines

SPECIAL TOPICS

4:50 PM

Frontiers of Materials Award Symposium: 2021 Functional Nanomaterials: Translating Innovation into Pioneering Technologies — Session IV

Program Organizer: Huanyu Cheng, Pennsylvania State University

Tuesday PM March 16, 2021

2:00 PM Invited Intelligent Materials at the AI-robotics-medicine Nexus: *Xuanhe Zhao*¹; ¹Massachusetts Institute of Technology

2:40 PM Invited Expansile Kirigami Wrapping Designs for Breast Reconstruction: Young-Joo Lee¹; Hyesung Cho¹; Jason Christopher Jolly¹; Eric Jablonka¹; Michael Tanis¹; Randall Kamien¹; Suhail Kanchwala¹; *Shu Yang*¹; ¹University of Pennsylvania

3:20 PM Invited Liquid Metals and Hydrogels: Inherently Stetchable Materials for Wearables: *Michael Dickey*¹; ¹North Carolina Stste University **MOBILE-FRIEND**



4:OO PM Invited Semiconductor Nanomaterials for Neural Interfaces: *John Rogers*¹; ¹Northwestern University

4:40 PM Invited Skin-inspired Organic Electronics: *Zhenan Bao*¹; ¹Stanford University

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Gradient Materials

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

Tuesday PM March 16, 2021

Session Chairs: Brad Boyce, Sandia National Lab; Hyoung Seop Kim, Postech; Suveen Mathaudhu, University of California, Riverside

2:00 PM Invited Chemical Gradients to Control Stability and Mechanical Behavior in

Nanostructured Pt-Au: *Brad Boyce*¹; David Adams¹; Khalid Hattar¹; Remi Dingreville¹; Riley Parrish¹; Fadi Abdeljawad²; ¹Sandia National Laboratories; ²Clemson University

Multi-layered Gradient Structure by Single-roll Angular-rolling and Ultrasonic Nanocrystalline Surface Modification: *Hyoung Seop Kim*¹; Hak Hyeon Lee¹; Hyung Keun Park¹; Jaimyun Jung²; Auezhan Amanov³; ¹Pohang University of Science and **TUESDAY PM**

2:45 PM

2:25 PM

Mechanical Enhancement of Graded Nanoporous Structure: Lijie He¹; Niaz Abdolrahim¹; ¹University of Rochester

3:05 PM

Tuning the Strongest Size by Tailoring Grain Size Gradient in Metals: Penghui *Cao*¹; ¹University of California Irvine

3:25 PM Invited

Technology; ²KIMS; ³Sun Moon University

Exploring the Grain Size Stability of Heterogeneous Copper in Thermal, **Mechanical and Radiation Environments**: Heather Salvador¹; Evander Ramos¹; Sina Shahrezaei²; Trevor Clark³; Khalid Hattar³; *Suveen Mathaudhu*¹; ¹University of California, Riverside; ²Pacific Northwest National Laboratory; ³Sandia National Laboratories

3:50 PM

Site-specific Texture Control for Functionally Graded Structures of Stainless Steel 316L Manufactured by Selective Laser Melting: Karl Sofinowski¹; Raman Sudharshan¹; Adarsh Nair¹; Matteo Seita¹; ¹Nanyang Technological University

MOBILE-FRIEND



High Entropy Alloys IX: Alloy Development and Properties — Alloy **Development and Application III**

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Tuesday PM March 16, 2021

Session Chairs: Wen Chen, University of Massachusetts Amherst; Duck Kim, Tennessee Technological University

2:00 PM Invited High-Entropy Alloys Containing Cu: Effects on Microstructure and Liquid Phase: Reza Abbaschian¹; *Nicholas Derimow*²; Raquel Jaime¹; Bryan Le¹; ¹University of California, Riverside; ²National Institute of Standards and Technology

2:25 PM Invited

Accelerated Design of High-entropy Alloys for Gas-Turbine Blade Components: Baldur Steingrimsson¹; Joseph Poon²; Michael Widom³; Anand Kulkarni⁴; Xuesong Fan⁵; Chanho Lee⁵; Chuan Zhang⁶; Michael Kirka⁷; Jaafar El-Awady⁸; *Peter Liaw*⁵; ¹Imagars LLC; Portland State University; ²University of Virginia; ³Carnegie Mellon University; ⁴Siemens Corporation; ⁵University of Tennessee; ⁶CompuTherm LLC; ⁷Oak Ridge National Laboratory; ⁸John Hopkins University



2:50 PM Invited **Effect of Process Parameters on the Microstructure and Mechanical Properties** of Wire+Arc Additively Manufactured AlCoCrFeNi High Entropy Alloy: Rumman Ahsan¹; Xuesong Fan²; Gi-Jeong Seo¹; Peter Liaw²; *Duck Bong Kim*¹; ¹Tennessee Technological University; ²The University of Tennessee, Knoxville

3:15 PM Invited Welding Metallurgy and Weld Properties of High Entropy Alloys: Carolin Fink¹; Alexander C. Martin¹; ¹Ohio State University

3:40 PM Invited Fabrication of Medium- and High-entropy Alloys Using Electroplating and Radio Frequency Plasma: Yu Zou¹; ¹University of Toronto

4:05 PM

Friction Stir Gradient Alloying: A Novel High-throughput Screening Technique to Explore HCP to BCC Transformation in a γ -FCC Dominated High Entropy Alloy by VAddition: Priyanka Agrawal¹; Shivakant Shukla¹; Sanya Gupta¹; Priyanshi Agrawal¹; Rajiv Mishra¹; ¹University of North Texas

4:25 PM

Exploring the Structure-property Relationships of (Ti, TiAl6V4)xCoCrFeMnNi Graded High Entropy Alloy: *Michael Melia*¹; Jonathan Pegues¹; Mark Rodriguez¹; Raymond Puckett¹; Shaun Whetten¹; Nicolas Argibay¹; Andrew Kustas¹; ¹Sandia National Laboratories



TUESDAY PM

MOBILE-FRIEND

High Entropy Alloys IX: Structures and Modeling - Structures and Characterization I

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Tuesday PM March 16, 2021

Session Chairs: Robert Ritchie, University of California, Berkeley; Michael Widom, Carnegie Mellon University

2:00 PM Invited Electronic Effects on the Mechanical Properties of HEA: Takeshi Egami¹; ¹University of Tennessee

2:25 PM Invited

An Averaged Cluster Approach to Include Chemical Short Range Order in First Principles Calculations with Application to High Entropy Alloys: Vishnu Raghuraman¹; Yang Wang¹; *Michael Widom*¹; ¹Carnegie Mellon University

2:50 PM

Faulting-mediated Plasticity in a CoCrNiW Complex Concentrated Alloy: Shaolou *Wei*¹; Cem Tasan¹; ¹Massachusetts Institute of Technology



3:10 PM Invited

Unique Deformation Behavior in the NbTaTiV Refractory High-entropy Alloy: *Chanho Lee*¹; George Kim²; Yi Chou³; Brianna Musicó¹; Michael Gao⁴; Ke An⁵; Gian Song⁶; Yi-Chia Chou³; Veerle Keppens¹; Wei Chen²; Peter Liaw¹; ¹University of Tennessee; ²Illinois Institute of Technology; ³National Chiao Tung University; ⁴National Energy Technology Laboratory/Leidos Research Support Team; ⁵Oak Ridge National Laboratory; ⁶Kongju National University

3:35 PM Invited

Unprecedented Supercritical Elasticity in NiCoFeGa Multi-principal-element Alloys: Haiyang Chen¹; Yan-Dong Wang¹; Yang Ren²; ¹University of Science and Technology Beijing; ²Argonne National Laboratory

4:00 PM Invited

Influence of Ductile Multicomponent Intermetallic Phase on Mechanical Behavior in High-entropy Alloys: Rui Feng¹; You Rao²; Huamiao Wang³; Yan Chen¹; Chuan Zhang⁴; Maryam Ghazisaeidi²; Ke An¹; Peter Liaw⁵; ¹Oak Ridge National Laboratory; ²The Ohio State University; ³Shanghai Jiao Tong University; ⁴Computherm, LLC; ⁵The University of Tennessee, Knoxville

MATERIALS PROCESSING

High Temperature Electrochemistry IV — Session III

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National



TUESDAY PM

CONTENTS

TABLE OF

Laboratory); Guy Fredrickson, Idaho National Laboratory

March 16, 2021 **Tuesday PM**

Session Chair: Michael Simpson, University of Utah

2:00 PM

Validated Modeling of Quartzite Reduction to Solar Silicon by Molten Salt Electrolysis: Aditya Moudgal¹; Mohammad Asadikiya¹; Jacob Hazerjian¹; Vicky Luu¹; Ariana Ly¹; Adam Powell¹; Uday Pal²; Yu Zhong¹; ¹Worcester Polytechnic Institute; ²Boston University

2:30 PM

A Comparative Study of Working Electrode Materials for Voltammetry Measurements in LiCl-Li2O Salts: Guoping Cao¹; Ammon Williams¹; Michael Shaltry¹; ¹Idaho National Laboratory

3:00 PM

Liquid Bipolar Electrode for Extraction of Aluminium and PGM Concentrate from **Spent Catalysts**: *Andrey Yasinskiy*¹; Peter Polyakov¹; Dmitriy Varyukhin¹; Sai Krishna Padamata¹; ¹Siberian Federal University

MATERIALS DESIGN

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session IV



Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

Tuesday PM March 16, 2021

Session Chair: Dana Frankel, QuesTek Innovations LLC

2:00 PM Invited High-throughput Synthesis, Characterization and Prediction of Metallic Glass Formation: John Perepezko¹; Janine Erickson¹; Dan Thoma¹; Carter Francis¹; Paul Voyles¹; Benjamin Afflerbach¹; Dane Morgan¹; ¹University of Wisconsin-Madison

2:40 PM Invited A Thermodynamic and Molar Volume Database for Co-base Superalloys: Ursula Kattner¹; Peisheng Wang²; ¹National Institute of Standards and Technology; ²Central South University

3:20 PM Invited Phase Stability and Kinetic Considerations in Materials Processing and Performance: *Steven Zinkle*¹; Yajie Zhao¹; Ty Austin¹; Ying Yang¹; ¹University of Tennessee

4:00 PM Invited Machine Learning-assisted ICME Approaches to Explore the Alloy and Process Space in Metals Additive Manufacturing: *Raymundo Arroyave*¹; ¹Texas A&M



University

4:40 PM Invited Printability and Properties of Metallic Alloys for Laser Powder Bed Fusion Additive Manufacturing: *Yongho Sohn*¹; Le Zhou¹; Holden Hyer¹; Abhishek Mehta¹; ¹University of Central Florida

LIGHT METALS

Magnesium Technology 2021 — Fundamentals of Plastic Deformation

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Petra Maier, University of Applied Sciences Stralsund; J. Brian Jordon, University of Alabama; Neale Neelameggham, IND LLC

Tuesday PM March 16, 2021

Session Chairs: Tracy Berman, University of Michigan; Sean Agnew, University of Virginia

2:00 PM Invited Accounting for the Effects of Dislocation Climb Mediated Flow in Mg alloy ZK10 Sheet: Michael Ritzo¹; Sean Agnew¹; ¹University of Virginia

2:30 PM

Three Dimensional Interaction of {101 ⁻2} Twins with Tilt Boundaries in Mg: Twin and Dislocation Transmission: Khanh Dang¹; John Graham¹; Carlos Tome¹; Vincent

Taupin²; *Laurent Capolungo*¹; ¹Los Alamos National Laboratory; ²LEM3

2:50 PM Invited **Revisiting <c+a> Pyramidal Slip in Magnesium**: Jaafar El-Awady¹; ¹Johns Hopkins University

3:20 PM

Thermally Activated Nature of Basal and Prismatic Slip in Mg and Its Alloys: Mohammed Shabana¹; Jishnu Bhattacharyya¹; Marek Niewczas²; Sean Agnew¹; ¹University of Virginia; ²McMaster University

3:40 PM

Mechanisms and Machine Learning for Magnesium Alloys Design: Zongrui Pei¹; ¹National Energy Technology Laboratory

4:00 PM

Three Dimensional Atomistic Simulations of {101 ⁻2} Non-cozone Twin -- Twin Interaction in Mg – Role of Twin Stability and Mobility: Khanh Dang¹; Carlos Tomé¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

NUCLEAR MATERIALS

Materials and Chemistry for Molten Salt Systems – Electrochemistry

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short,



TUESDAY PM

CONTENTS

TABLE

Q

Massachusetts Institute of Technology; Raluca Scarlat, University of California-Berkeley

Tuesday PM March 16, 2021

Session Chair: Nathaniel Hoyt, Argonne National Laboratory

2:00 PM

Research Paths on Spectroelectrochemistry for Molten Salt Chemistry in the U.S. with Respect to Other Nations: Supathorn Phongikaroon¹; ¹Virginia Commonwealth University

2:30 PM

Materials Compatibility and Potential Stability of Reference Electrodes for Molten FLiBe: Francesco Carotti¹; Raluca Scarlat²; ¹University of Wisconsin, Madison; ²University of California, Berkeley

2:50 PM

Redox Measurement and Control in Molten Chloride Fast Reactor Fuel Salt: *Matthew Newton*¹; D. Hamilton¹; Michael Simpson¹; ¹Univ of Utah

3:10 PM

Oxidation Potential of Molten Halide Salts: A First Principles Study: *Jianguo Yu*¹; Guoping Cao¹; ¹Idaho National Lab

3:30 PM

High-throughput Electrochemical Characterization and Screening of CSPrelevant Alloys: Nathaniel Hoyt¹; Jicheng Guo¹; Mark Williamson¹; ¹Argonne National Laboratory



MOBILE-FRIENDL

3:50 PM

Corrosion of Zircaloy-2 in Molten LiCl-xLi2O at 650 °C: *Vineeth Kumar Gattu*¹; Evan Wu¹; William Ebert¹; ¹Argonne National Laboratory

4:10 PM

Development of an Electrochemical Phase Field Model for the Corrosion of Ni-Cr Alloys by Molten Fluoride Salts: *Chaitanya Bhave*¹; Michael Tonks¹; David Andersson²; Jake McMurray³; ¹University of Florida; ²Los Alamos National Laboratory; ³Oak Ridge National Lab

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Metallurgy

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao, University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology Company Ltd.; Shadia Ikhmayies

Tuesday PM March 16, 2021

Session Chairs: Ailiang Chen, Central South University; Xiaodi Huang, Michigan



TUESDAY PM

TABL

Π

Q

NTENTS

2:00 PM Invited Effect of Boron Iron Concentrate on the Strength of Preheated Iron Ore Pellets: Li Ma¹; *Gele Qing*; Zhixing Zhao¹; Baojun Zhao²; ¹Shougang Research Institute of Technology; ²University of Queensland

2:20 PM

Metallographic Feature of a Nickel-based Superalloy in Fluoride Electrolyte Melt: *Bowen Li*¹; Xiaodi Huang¹; Jiann-Yang Hwang¹; ¹Michigan Technological University

2:40 PM Invited

Phase Diagram and Thermodynamic Properties of Cu-O Binary System: Shadia Ikhmayies

3:00 PM

Characterization of Mixing Conditions of Different Nozzle and Porous Plugs Setups in Non-ferrous Refining Furnaces: *Anton Ishmurzin*¹; Daniel Kreuzer¹; Goran Vukovic¹; ¹RHI Magnesita

3:20 PM Invited

The Formation Mechanism of the Third Phase in Nickel Electrolyte: *Ailiang Chen*¹; Jiale Mao¹; Guanwen Luo¹; Sujun Lu²; Peng Zhang³; Yutian Ma³; Shengli Chen²; Zuojuan Du¹; Jinxin Qiao¹; Bowen Li⁴; ¹Central South University; ²State Key Laboratory of Nickel and Cobalt Resources Comprehensive Utilization, Jinchang; ³State Key Laboratory of Nickel and Cobalt Resources Comprehensive Utilization, Jinchang; Jinchang ; ⁴Michigan Technological University

Materials for High Temperature Applications: Next Generation Superalloys and

Beyond — Refractory Alloys: Design and Mechanical Properties

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Tuesday PM March 16, 2021

2:00 PM Invited

Rapid Screening, Machine Learning, and Multi-objective Optimization for **Refractory Alloy Development**: Andrew Detor¹; Meinolf Sellmann¹; Scott Oppenheimer¹; Emily Cheng¹; James Ruud¹; ¹GE Research

2:30 PM

Rapid Design of Refractory Multi-principal Element Alloys for High-T Structural Applications: Theory-guided Combinatorial Synthesis and Characterization Approach: Gaoyuan Ouyang¹; Prashant Singh¹; Ranran Su²; Shalabh Gupta¹; John Perepezko²; Jun Cui¹; Matthew Kramer¹; Duane Johnson¹; ¹Ames Laboratory (US) DOE); ²University of Wisconsin – Madison

2:50 PM

New Tools for Analysis of Microplasticity in BCC Refractory Metals: Leah Mills¹;



Jean-Charles Stinville¹; Marie-Agathe Charpagne¹; Joseph Wendorf¹; McLean Echlin¹; Valéry Valle²; Paul Dawson³; Daniel Gianola¹; Tresa Pollock¹; ¹University of California Santa Barbara; ²Pprime Institut; ³Cornell University

3:10 PM

The Creep Performance of Pesting-Resistant Mo-Si-Ti Alloys: Susanne Obert¹; Alexander Kauffmann¹; Martin Heilmaier¹; ¹Karlsruhe Institute for Technology

3:30 PM

Effect of Processing Parameters on Molybdenum Weld Microstructures: Noah *Kohlhorst*¹; Govindarajan Muralidharan²; Roger Miller²; Kevin Faraone²; Ji-Cheng Zhao³; ¹Ohio State Univerity; ²Oak Ridge National Laboratory (ORNL); ³University of Maryland, Department of Materials Science and Engineering

3:50 PM

Creep Testing of Molybdenum: Brandon Kenny¹; Jacqueline Foradora²; Alex Xie³; *Gary Rozak*²; ¹Miami University; ²H.C. Starck Solutions Euclid; ³H.C. Starck Solutions Taicang

MATERIALS PROCESSING

Materials Processing Fundamentals — Steel Casting



Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Process Technology and Modeling Committee

Program Organizers: Jonghyun Lee, Iowa State University; Samuel Wagstaff, Oculatus; Alexandra Anderson, Gopher Resource; Fiseha Tesfaye, Abo Akademi University; Guillaume Lambotte, Boston Metal; Antoine Allanore, Massachusetts Institute of Technology

Tuesday PM March 16, 2021

Session Chairs: Samuel Wagstaff, Oculatus Consulting; Antoine Allanore, MIT

2:00 PM

The CuCl₂-CuSO₄-ZnSO₄ System at Elevated Temperatures: *Fiseha Tesfaye*¹; Daniel Lindberg²; Mykola Moroz³; Leena Hupa¹; ¹Abo Akademi University; ²Aalto University; ³Ivan Franko National University of Lviv

2:20 PM

Stress Development Simulation in Continuously Cast Steel Slabs during Cooling Process: Duo Huang¹; ¹Purdue University

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Microstructure Effects

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS



Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory

Tuesday PM March 16, 2021

2:00 PM

He Ion Irradiation Response of a Gradient T91 Steel: *Zhongxia Shang*¹; Jie Ding¹; Cuncai Fan²; Di Chen³; Jin Li¹; Yifan Zhang¹; Yongqiang Wang⁴; Haiyan Wang¹; Xinghang Zhang¹; ¹Purdue University; ²Oak Ridge National Laboratory; ³University of Houston; ⁴Los Alamos National Laboratory

2:20 PM

High Temperature Strength of Additively Manufactured Gr91 Steel: *Benjamin Eftink*¹; Daniel Vega²; Osman El Atwani¹; David Sprouster³; Carl Cady¹; Mohamad Al-Sheikhly⁴; Thomas Lienert⁵; Stuart Maloy¹; ¹Los Alamos National Laboratory; ²DOE; ³Stony Brook University; ⁴University of Maryland; ⁵T.J. Lienert Consulting, LLC

2:40 PM Invited

Wear Behavior of Incoloy[™] 800HT and Inconel[™] 617 for High-Temperature Gas-cooled Reactor (HTGR) Applications: Valentin Pauly¹; Joseph Kern¹; Malcolm Clark¹; David Grierson¹; *Kumar Sridharan*¹; ¹University of Wisconsin-Madison

3:10 PM

Modeling the Effect of Helium Bubbles, Rigid Inclusions, and Grain Boundaries on Crack Initiation in Nickel: *Tung Yan Liu*¹; Michael Demkowicz¹; ¹Texas A&M

University

3:30 PM

Quantifying Zirconium Embrittlement Due to Hydride Microstructure Using Image Analysis: *Pierre-Clement Simon*¹; Cailon Frank¹; Long-Qing Chen¹; Mark Daymond²; Michael Tonks³; Arthur Motta¹; ¹The Pennsylvania State University; ²Queen's University; ³University of Florida

3:50 PM

In-situ Observations of the Failure Mechanisms of Hydrided Zircaloy-4 under Different Stress-States: Brian Cockeram¹; Kwai Chan²; ¹Naval Nuclear Laboratory-Bettis Laboratory; ²Southwest Research Institute

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ **Experiments and Modeling — Session IV**

Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

MOBILE-FRIENDL

March 16, 2021 **Tuesday PM**

Session Chair: Amit Pandey, Lockheed Martin Space

2:00 PM

Quantifying the Long-range Stress ahead of the Tip of a Dislocation Pileup at a Grain Boundary and Its Contribution to the Subsequent Structure Changes in Tialloys from the Atomistic to the Mesoscale: Liming Xiong¹; ¹Iowa State University

2:20 PM

Dislocation Pileup Induced Transmission across Grain Boundaries in Aluminum via Molecular Dynamics Simulations: Royce Reyes¹; Douglas Spearot¹; ¹University of Florida

2:40 PM

Decoupling the Effect of Nanoscale Geometry and Internal Microstructure on the Mechanics of Nanoporous Pt: Ankit Gupta¹; Timothy Ibru²; Antonia Antoniou²; *Garritt Tucker*¹; ¹Colorado School Of Mines; ²Georgia Institute of Technology

3:00 PM

Constitutive Model Materials Parameter Determination Using Cyclic Tensioncompression Test Data: *Dilip Banerjee*¹; William Luecke¹; Mark Iadicola¹; Evan Rust¹; ¹National Institute of Standards and Technology

3:20 PM

Multiphysics Modeling of Coupled Chemical-Thermal-mechanical Phenomena in Chemically Blown Polyurethane Foams during Manufacturing: Kevin Long¹; Judith Brown¹; Rekha Rao¹; Christine Roberts¹; ¹Sandia National Laboratories



2:00 PM Effective Treatment of Domestic US Cobalt Ores and Concentrates: Andy Tomaka¹;

3:40 PM

Effects of Phase Purity and Pore-reinforcement on the Mechanical Behavior of Metal-organic Frameworks: Kevin Schmalbach¹; Zhao Wang¹; Rebecca Combs¹; Youxing Chen²; R. Lee Penn¹; Andreas Stein¹; Nathan Mara¹; ¹University of Minnesota; ²University of North Carolina at Charlotte

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — Hydrometallurgy II

Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

March 16, 2021 **Tuesday PM**

TABLE NTENTS **P**





TUESDAY PM

*Corby Anderson*¹; ¹Colorado School of Mines

2:20 PM Separating and Recovering Cobalt and Iron from Co, Fe-bearing Metallurgical Slag via Acid Leaching Process: Yuanbo Zhang¹; Yikang Tu¹; Zijian Su¹; Tao Jiang¹; ¹Central South University

2:40 PM Starved Acid Leaching Technology for Nickel and Cobalt Recovery from Lean **Resources**: *David Dreisinger*¹; ¹University of British Columbia

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Ferrous Alloys

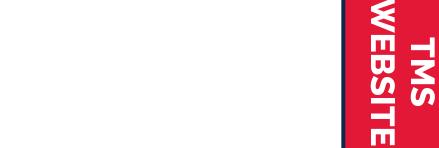
Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno ; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos

National Laboratory

Tuesday PM March 16, 2021

Session Chair: HuaJing Song, Los Alamos National Lab



2:00 PM

Solute Partitioning during the Double Soaking Heat Treatment of Medium Manganese Steels: *Alexandra Glover*¹; Emmanuel De Moor²; John Speer²; ¹Los Alamos National Laboratory; ²Colorado School of Mines

2:20 PM

CementiteFormationinFerriticSteels:Ffirst-principlesBasedAtomisticSsimulations.:OcéaneBuggenhoudt¹;Chu-Chun Fu¹;ThomasSchuler¹;Jean-Luc Béchade¹;¹CEA, Université Paris Saclay

2:40 PM

Effect of Cold Rolling on PhaseTtransformations in 2202 Lean Duplex Stainless Steel: *Frederic Danoix*¹; Sophie Cazottes²; Raphaele Danoix³; Dimitri Rolland²; Sarata Cissé⁴; Véronique Massardier²; ¹CNRS; ²INSA Lyon; ³CNRS - Univ Rouen Normandie; ⁴INDUSTEEL

3:00 PM

Phase Instability and Formation of Radiation-induced BCC-phases in Austenitic Stainless Steel after Long Term Neutron Exposure: Diana Merezhko¹; *Mikhail Merezhko*¹; Maxim Gussev²; Thomas Rosseel²; Oleg Maksimkin¹; Francis Garner³; ¹Institute of Nuclear Physics; ²Oak Ridge National Laboratory; ³Radiation Effects Consulting

3:20 PM

Applicability of Deep Cryogenic Treatment in Emerging Industries: *Patricia Jovicevic-Klug*¹; Matic Jovicevic-Klug¹; Bojan Podgornik¹; ¹Institute of Metals and Technology

2021 TUESDAY PM

TABLE

P

NTENTS

Austempered Microstructures for Bearing Applications: *Scott Hyde*¹; ¹The Timken Company

MATERIALS PROCESSING

Rare Metal Extraction & Processing — REEs, Sc

Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

Tuesday PM March 16, 2021

2:00 PM Keynote Understanding the Feasibility for Secondary and by Product Sources to Supply Rare Earth Metals: *Gabrielle Gaustad*¹; Eric Williams²; Alexandra Leader²; Ajay Gupta²; Saptarshi Das²; ¹Alfred University; ²Rochester Institute of Technology

2:20 PM Invited Uranium and Thorium Removal from Rare Earth Sulfate Solutions by Ion Exchange and Solvent Extraction: *David Dreisinger*¹; Mike Johnson²; Niels Verbaan²; Greg Andrews²; ¹University of British Columbia; ²SGS Minerals

2:40 PM Invited

Rare Earth Elements Extraction from Coal Waste Using Biooxidation Approach:

*Prashant Sarswat*¹; Michael Free¹; ¹University of Utah



3:00 PM Invited

Supercritical Extraction of Neodymium from NdFeB Using Magnet **Organophosphorus Ligands**: Nattanai Kunanusont¹; Jiakai Zhang²; Kimberly Watada²; Yusuke Shimoyama¹; *Gisele Azimi*²; ¹Tokyo Institute of Technology; ²University of Toronto

3:20 PM Invited

Scandium Extraction from Bauxite Residue Using Sulfuric Acid and a Composite **Extractant-enhanced Ion-exchange Polymer Resin**: *Efthymios Balomenos*¹; Ghazaleh Nazari²; Panagiotis Davris¹; Gomer Abrenica²; Anastasia Pilichou³; Eleni Mikeli³; Dimitrios Panias³; Shailesh Patkar²; Wen-Qing Xu²; ¹Mytilineos Metallurgy Buisness Unit; ²II-VI; ³NTUA

3:40 PM Invited Scandium: Leaching and Extraction Chemistry: Dag Eriksen¹; ¹Primus.Inter.Pares As

4:00 PM Invited **Environmentally Friendly Solid Phase Extraction of Critical Materials and REE** from Unconventional Sources: Athanasios Karamalidis¹; Jonathan Callura²; Madhav Patel¹; ¹Pennsylvania State University; ²Carnegie Mellon University

ENERGY & ENVIRONMENT

Recycling and Sustainability for Emerging Technologies and Strategic Materials — E-Waste & Value Recovery

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals



TUESDAY PM

Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: John Howarter, Purdue University; Mingming Zhang, ArcelorMittal Global R&D; Elsa Olivetti, Massachusetts Institute of Technology; Hong Peng, University of Queensland

Tuesday PM March 16, 2021

Session Chair: John Howarter, Purdue University

2:00 PM Invited Characterisation and Techno-economics of a Process to Recover Value from **E-waste Materials**: *Khairul Islam*¹; Michael Somerville²; Nawshad Haque²; ¹RMIT University; ²CSIRO

2:30 PM

Recycling of Spent SCR Catalyst to Recover Vanadium and Tungsten by Hydrometallurgical Routes: Ana Belen Cueva-Sola¹; Jin-Young Lee²; Rajesh Kumar Jyothi²; ¹Korea University of Science and Technology (UST), Daejeon 34113, South Korea; ²Korea Inst of Geoscience & Mineral Resources

2:50 PM

The Separation of Nickel and Cobalt from Lithium-ion Battery Leachate: Mark *Strauss*¹; Josh McNally¹; Luis Aldana¹; John Klaehn¹; Tedd Lister¹; ¹Idaho National Laboratory

3:10 PM

Rare Earth Magnet or Ferroalloy? What Steel Processing Can Teach Us about Magnet Sludge Recycling.: Mary Elizabeth Wagner¹; Antoine Allanore¹; ¹Massachusetts Institute of Technology





100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture and Cracks

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

Wednesday AM March 17, 2021

Session Chair: Nathan Mara, University of Minnesota

8:30 AM Invited Modeling Mechanics of Nanoparticles: Everything but Size: Jonathan Amodeo¹; Laurent Pizzagalli²; ¹MATEIS lab, INSA-Lyon Univ. Lyon CNRS; ²P' institute, Univ. **Poitiers CNRS**

9:10 AM

The Curious Phenomenon of Prince Rupert's Drops: Koushik Viswanathan¹; Hillar Aben²; Munawar Chaudhri³; *Srinivasan Chandrasekar*⁴; ¹Indian Institute of Science; ²Tallinn University of Technology; ³University of Cambridge; ⁴Purdue University

9:30 AM Effect of Aspect Ratio on Stress Intensity Factor Solutions for Single Edge Notch Wire Fracture Test Specimen under Tensile and Clamped Bend Loading **Conditions**: *Hrushikesh Sahasrabuddhe*¹; Ashwini Mishra¹; Nagamani Jaya Balila¹; ¹India Institute of Technology Bombay

ADVANCED MATERIALS

2D Materials – Preparation, Properties & Applications – Case Studies & **Applications**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Sufian Abedrabbo, Khalifa University; Amber Shrivastava, Indian Institute of Technology Bombay

Wednesday AM March 17, 2021

Session Chairs: Amber Shrivastava, Indian Institute of Technology; Ramana Chintalapalle, University of Texas - El Paso

8:30 AM Invited Formation of h-BN Ultrathin Films and Heterojunction MIS Diodes by Pulsed Laser **Annealing**: *Siddharth Gupta*¹; Ritesh Sachan²; Jagdish Narayan¹; ¹North Carolina State University; ²Oklahoma State University



WEDNESDAY AM TABLE **ONTENTS**

Q

8:55 AM Invited Graphene and Carbon Nanotubes: Key Materials for Electrochemical Energy Materials and Nano Biosensors: Eon Soo Lee¹; ¹New Jersey Institute of Technology

9:20 AM Invited **hBN for Quantum Information Sciences**: *Ritesh Sachan*¹: ¹Oklahoma State University

9:45 AM

The Growth of NbSe, by Molecular Beam Epitaxy for Thermomagnetic Energy **Conversion**: *Peter Litwin*¹; Sabbir Akhanda¹; Mona Zebrajadi¹; Stephen McDonnell¹; ¹University of Virginia

NUCLEAR MATERIALS

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — Data Analytics and Machine Learning in Nuclear Energy **Applications**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University



Wednesday AM March 17, 2021

Session Chairs: Dane Morgan, University of Wisconsin; Karim Ahmed, Texas A&M U

8:30 AM Invited Machine Learning and Atomistic Modeling of Defect Diffusion in Concentrated **Ni-Fe Alloys**: Wenjiang Huang¹; *Xian-Ming Bai*¹; ¹Virginia Polytechnic Institute and State University

9:00 AM

Characterization of As-Fabricated Additively Manufactured Alloy 718 Enhanced by Modern Tools and Machine Learning: Stephen Taller¹; Luke Scime¹; Kurt Terrani¹; ¹UT-Battelle

9:20 AM Invited

Machine Learning for Accelerating Property Prediction and Materials Characterization in Irradiated Materials: Dane Morgan¹; Mingren Shen¹; Ryan Jacobs¹; G. Robert Odette²; Kevin Field³; ¹University of Wisconsin-Madison; ²University of California, Santa Barbara; ³University of Michigan

9:50 AM

Point Defect Energies in Concentrated Alloys Using Ab Initio Calculations and Machine Learning: Anus Manzoor¹; Gaurav Arora¹; Dilpuneet Aidhy¹; ¹University of Wyoming

10:10 AM Invited

Machine Learning Perovskites in the Quest for Improved Scintillators: Anjana Talapatra¹; Christopher Stanek¹; Blas Uberuaga¹; *Ghanshyam Pilania*¹; ¹Los Alamos

National Laboratory

10:40 AM

An Integrated Approach for Coupling Experimental Data, Physics-based Models, and Machine Learning Algorithms for Predicting the Effective Thermal **Conductivity of U-based Fuels**: *Karim Ahmed*¹; Fergany Badry¹; ¹Texas A&M University

11:00 AM

Deep Learning for Automated Analysis of Cavities in Transmission Electron Microscopy Images: Chun Yin Wong¹; Xing Wang²; Zhe Fan³; Karren More⁴; Sergei Kalinin⁴; Maxim Ziatdinov⁴; ¹University of Tennessee; ²The Pennsylvania State University, Oak Ridge National Laboratory; ³Lamar University, Oak Ridge National Laboratory; ⁴Oak Ridge National Laboratory

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Fatigue Modeling and **Prediction**

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Wednesday AM March 17, 2021



WEDNESDAY AM

8:30 AM Invited Damage Tolerant Approach in Additively Manufactured Metallic Materials: Mauro *Madia*¹; Uwe Zerbst¹; Tiago Werner¹; ¹Bundesanstalt fuer Materialforschung und -pruefung (BAM)

9:00 AM

Defect-based Fatigue Model for AlSi10Mg Produced by Laser Powder Bed Fusion **Process**: Avinesh Ojha¹; Wei-Jen Lai¹; Ziang Li¹; Carlos Engler-Pinto Jr.¹; Xuming Su¹; ¹Ford Motor Company

9:20 AM

State-of-the-Art in Predicting Fatigue Life for Applications in Metal-based Additive Manufacturing: Newell Moser¹; Orion Kafka¹; Jake Benzing¹; Nicholas Derimow¹; Nik Hrabe¹; Edward Garboczi¹; ¹National Institute of Standards and Technology

9:40 AM Invited Synergistic Effects of Defects and Microstructure on Fatigue Behavior of LB-PBF Metallic Materials: Shuai Shao¹; Nima Shamsaei¹; ¹Auburn University

10:10 AM

Microstructure-based Model Validation and Predictions of Single-build-plate Fatigue Strength Sensitivity for Additively Manufactured Ti-6Al-4V: Orion *Kafka*¹; Newell Moser¹; Jake Benzing¹; Nicholas Derimow¹; Nikolas Hrabe¹; Edward Garboczi¹; ¹NIST

10:30 AM

3-D Convolutional Neural Networks for Pore Analysis in Metal Additive Manufacturing Builds: Andrew Kitahara¹; Ziheng Wu¹; Srujana Yarasi¹; Nihal

Session Chair: Paul Prichard, Kennametal

8:30 AM Introductory Comments: Additive Manufacturing: Beyond the Beam II: Paul Prichard¹; ¹Kennametal Inc.

Sivakumar¹; Anthony Rollett¹; Elizabeth Holm¹; ¹Carnegie Mellon University

10:50 AM

Bayesian Inference of Elastic Constants and Texture Coefficients in Additively Manufactured Alloys Using Resonant Ultrasound Spectroscopy: Jeffrey Rossin¹; Patrick Leser²; Chris Torbet¹; Stephen Smith²; Samantha Daly¹; Tresa Pollock¹; ¹University of California, Santa Barbara; ²NASA Langley Research Center

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Beyond the Beam II — Binder Jetting

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Paul Prichard, Kennametal Inc.; James Paramore, US Army Research Laboratory; Peeyush Nandwana, Oak Ridge National Laboratory; Nihan Tuncer, Desktop Metal

Wednesday AM March 17, 2021



MOBILE-FRIEND

8:35 AM

A Look into Solid-state Metal AM Techniques from Metallurgical Bonding **Perspective**: *Nihan Tuncer*¹; Animesh Bose¹; ¹Desktop Metal

8:55 AM

Development, Characterization, and Modeling of a 3D Binder-jet Printed N95 Metal Filter for COVID-19: Aaron Acierno¹; Katerina Kimes¹; Erica Stevens¹; Pierangeli Rodriguez¹; Steve Pilz²; Kyle Myers³; Patrick Dougherty³; Kurt Svihla²; Thomas Spirka⁴; Markus Chmielus¹; ¹University of Pittsburgh; ²ANSYS; ³ExOne; ⁴Synopsys

9:15 AM

Effect of Processing Defects on Properties of Binderjet WC-Co: Paul Prichard¹; Hadi Miyanaji¹; Zhuqing Wang¹; ¹Kennametal Inc.

9:35 AM

Droplet Powder Interactions in Binder Jet Additive Manufacturing: Trenton Colton¹; *Nathan Crane*¹; ¹Brigham Young University

9:55 AM

Fluid and Particle Dynamics Simulation in Binder Jetting Process: Fangzhou Li¹; Wenda Tan¹; ¹University of Utah

10:15 AM

Gravity Influence on Sintering of Binder Jetted Components: Elisa Torresani¹; Eugene Olevsky¹; Randall German¹; ¹San Diego State University

10:35 AM

Distortion Modeling of Sintering Process in Binder Jet Printed Parts: Basil Paudel¹; Dave Conover²; Albert To¹; ¹University of Pittsburgh; ²ANSYS Inc.

TMS

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Materials Design and Alloy Development III -- Super Materials and Extreme Environments — Other Materials and Aspects

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek Innovations LLC

Wednesday AM March 17, 2021

Session Chair: Jiadong Gong, QuesTek

8:30 AM Invited Design of Novel Fe-based Bulk Metallic Glasses Enabled by Additive Manufacturing: Martin Walbrühl¹; Jiayi Yan¹; Ida Berglund¹; Zaynab Mahbooba²; Abhinav Saboo²; ¹QuesTek Europe AB; ²QuesTek Innovations

9:00 AM

Understanding the Corrosion Mechanism of an Equimolar AlCoCrFeNi Highentropy Alloy Additively Manufactured by Electron Beam Melting: Kenta Yamanaka¹; Hiroshi Shiratori²; Manami Mori³; Kazuyo Omura¹; Tadashi Fujieda²; Kosuke Kuwabara²; Akihiko Chiba¹; ¹Tohoku University; ²Hitachi, Ltd.; ³National Institute of Technology, Sendai College



Design and Additive Manufacturing of Hastelloy C22 for Corrosive Environment: Somayeh Pasebani¹; Dongqing Yan¹; Alireza Torbati-Sarraf²; Behrang Poorganji³; Osman Ertorer⁴; O Isgor¹; ¹Oregon State University; ²LAM Research Corporation and University of Southern California; ³University of Waterloo; ⁴Oryx Advanced Materials, Inc

9:40 AM

Catalytic Inhibition of Metal Dusting by Cu – The Difference of Cast and AM **Alloys**: *Anke Ulrich*¹; Clara Schlereth¹; Katrin Jahns²; Ulrich Krupp³; Mathias Galetz¹; ¹DECHEMA-Forschungsinstitut; ²University of Applied Sciences Osnabrück; ³RWTH Aachen University

10:00 AM

Correlating Data from Digital and Virtual Twins of Component Manufacturing via **DED**: Monica Salgueiro¹; Carlos Gonzalez¹; Camilo Prieto¹; Bernardo Freire²; Mihail Babcinschi²; Joerg Willem³; *Mustafa Megahed*³; ¹AIMEN; ²University of Coimbra; ³ESI Group

10:20 AM Material Development Using RF Plasma: Nicolas Gobeil¹; ¹Tekna

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Steels



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

March 17, 2021 Wednesday AM

Session Chairs: Eric Lass, The University of Tennessee Knoxville; Peeyush Nandwana, Oak Ridge National Laboratory

8:30 AM

The Crystallography and Orientation of Cellular Features in Additively Manufactured 316L: *Richard Fonda*¹; Joseph Aroh²; Jerry Feng¹; David Rowenhorst¹; ¹Naval Research Laboratory; ²Carnegie Mellon University

8:50 AM

The Dislocation and Composition Microstructure Evolution and Mechanical **Properties of Selective Laser Melted Stainless Steels**: *Markus Sudmanns*¹; Yejun Gu¹; Jaafar El-Awady¹; ¹Johns Hopkins University

9:10 AM

Microstructural Characterization of Maraging 300 Steel Fabricated by Select



Laser Melting: Johnnatan Rodriguez¹; Elizabeth Hoyos¹; Fabio Conde²; André Jardini Munhoz³; Julian Avila⁴; ¹EIA University; ²University of Sao Paolo; ³BIOFABRIS -National Institute of Science and Technology in Biomanufacturing; ⁴UNESP – São Paulo State University

9:30 AM

Recrystallization-based Grain Boundary Engineering of 316L Stainless Steel Produced via Selective Laser Melting: Shubo Gao¹; Zhiheng Hu²; Sravya Tekumalla¹; Matteo Seita¹; ¹Nanyang Technological University; ²Singapore Institute of Manufacturing Technology

9:50 AM Invited Grain Orientation Analysis of Additively Manufactured 316L Stainless Steel: Anthony Rollett¹; ¹Carnegie Mellon University

10:20 AM

Phase Transformation Modeling of Functionally Graded Materials Made by **Direct Energy Deposition**: *Noah Sargent*¹; Wei Xiong¹; Richard Otis²; ¹University of Pittsburgh; ²Jet Propulsion Laboratory

10:40 AM

Effect of Low-temperature Plasma Nitriding on the Wear and Corrosion Resistance of Additive-manufactured Stainless and Maraging Steels: Matjaz Godec¹; Crtomir Donik¹; Aleksandra Kocijan¹; Bojan Podgornik¹; Danijela Anica Skobir Balantic¹; ¹Institute of Metals and Technology

11:00 AM

Section Thickness Dependent Behavior in Additively Manufactured Stainless **Steel**: *Thomas Slagle*¹; Alexandra Vyatskikh¹; Sen Jiang¹; Salma El-Azab¹; Umberto Scipioni Bertoli¹; Lorenzo Valdevit¹; Enrique Lavernia¹; Julie Schoenung¹; ¹University of California Irvine



CHARACTERIZATION



AB

Π

O

NIENIS

Advanced Characterization Techniques for Quantifying and Modeling **Deformation – Session V**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Wednesday AM March 17, 2021

8:30 AM Invited

Combining Advanced Characterization Techniques to Rationalize the Multiple **Mechanical Behaviors Observed in TRIP/TWIP Ti-alloys**: Lola Lilensten¹; Yolaine Danard²; Inès Danard¹; Raphaëlle Guillou³; Nathalie Bozzolo⁴; Dominique Thiaudière⁵; Frédéric Prima¹; ¹CNRS - IRCP; ²ICMPE; ³CEA; ⁴Mines ParisTech - CEMEF ; ⁵Synchotron Soleil

9:00 AM

A Study on Migrating Boundary Induced Plasticity Using Atomistic Simulation:

*Simoon Sung*¹; Jaehoon Jang²; Hyerim Hwang³; Yanghoo Kim⁴; Heung Nam Han¹; ¹SeoulNationalUniversity; ²KoreaInstituteofMaterialsScience; ³HarvardUniversity; ⁴Korea Institute of Industrial Technology

9:20 AM

Deformation Behavior and Phase Transformation of Nanotwinned Al/Ti **Multilayers**: *Yifan Zhang*¹; Qiang Li¹; Mingyu Gong²; Sichuang Xue¹; Jie Ding¹; Jaehun Cho¹; Tongjun Niu¹; Ruizhe Su¹; Nicholas Richter¹; Haiyan Wang¹; Jian Wang²; Xinghang Zhang¹; ¹Purdue University; ²University of Nebraska-Lincoln

9:40 AM

Fingerprinting Shock-induced Deformations via Virtual Diffraction: Avanish *Mishra*¹; Cody Kunka²; Marco Echeverria¹; Rémi Dingreville²; Avinash Dongare¹; ¹University of Connecticut; ²Sandia National Laboratories

10:00 AM Invited

Deformation Behaviour of High-alloy Twinning-induced Plasticity Steels Unravelled by Complementary Local and Integral Methods: Stefan Martin¹; Christiane Ullrich¹; Christian Schimpf¹; Mykhaylo Motylenko¹; Anja Weidner¹; Horst Biermann¹; David Rafaja¹; Alexey Vinogradov²; Yuri Estrin³; ¹Tu Bergakademie Freiberg; ²NTNU; ³Monash University

10:30 AM

Ultrasonic Effects on Plastic Deformation Behavior of TRIP 780 Steel: *Jiarui Kang*¹; Xun Liu¹; ¹The Ohio State University

10:50 AM

In-situ Shock Stress Field Detection Using Laser Array Raman Spectroscopy: Abhijeet Dhiman¹; Ayotomi Olokun¹; Nolan Lewis¹; Vikas Tomar¹; ¹Purdue University

11:10 AM

Experimental Characterization and FFT-based Modeling of Heterogeneous

Deformation in HCP Materials: *Behnam Ahmadikia*¹; Leyun Wang²; Irene Beyerlein¹;

¹University of California, Santa Barbara; ²Shanghai Jiao Tong University

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Multifunctional **Biomaterials, Innovative Approaches to New Concepts and Applications I**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

Wednesday AM March 17, 2021

Session Chair: Adele Carrado, Université de Strasbourg IPCMS

8:30 AM Keynote Bio-inspired Nano- and Microstructured Surfaces: Hendrik Hoelscher¹; ¹Karlsruhe Institute of Technology

9:10 AM Invited TiN and DLC Coated Medical Grade Polyurethane (PUR) for Controlled Surface **Degradation and Improved Mechanical Properties**: *Maren Fossum*¹; Mohammad Ibrahim¹; Javier Sanchez²; Christoph Burgstaller³; Emma Strömberg⁴; Gunilla Björling⁵; Ragnhild Aune¹; ¹Norwegian University of Science and Technology; ²Danderyd Hospital at Karolinska Institute ; ³TCKT - Transfercenter für Kunststofftechnik GmbH; ⁴KTH Royal Institute of Technology; ⁵The Swedish Red Cross University College



9:40 AM Invited Multimodal Flexible Optoelectronic Devices for Colocalized Electrophysiology and Optophysiology: Luyao Lu¹; ¹George Washington University

10:10 AM Invited Structural and Biological Properties of Silicon-incorporated Diamond-like **Carbon Coatings**: *Roger Narayan*¹; ¹University of North Carolina

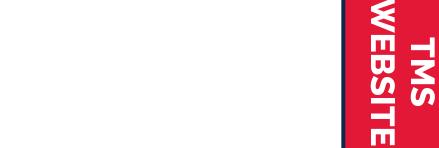
10:40 AM

Silicone Breast Implants: Grafting of a Bioactive Polymer to Improve the Biointegration: Mylan Lam¹; Vivien Moris¹; Vincent Humblot²; Véronique Migonney¹; Céline Falentin-Daudré¹; ¹Université Sorbonne Paris Nord; ²Université Bourgogne Franche-Comté

11:00 AM Keynote Determining the Interaction between Porous Titanium and Adhesion of a **Bioactive Coating**: *Holly Martin*¹; Patrick McWhorter¹; Arthur Kasson¹; Snjezana Balaz¹; ¹Youngstown State University

ENERGY & ENVIRONMENT

Advanced Magnetic Materials for Energy and Power Conversion Applications - Structures and Modelling of Soft Magnetic Materials



Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

Wednesday AM March 17, 2021

Session Chair: Richard Beddingfield, North Carolina State University

8:30 AM Invited

Advanced Magnetics for Power and Energy Development (AMPED) : A New Consortium Model for US Power Magnetics Research and Workforce **Development**: *Paul Ohodnicki*¹; Brandon Grainger¹; Michael McHenry²; Maarten DeBoer²; Subhashish Bhattacharya³; Richard Beddingfield³; ¹University of Pittsburgh; ²Carnegie Mellon University; ³North Carolina State University

9:00 AM

Radio Frequency Rapid Thermal Processing of Nanocrystalline Soft Magnetic Alloys: Ahmed Talaat¹; David Greve²; *Paul Ohodnicki*¹; ¹University of Pittsburgh; ²DWGreve Consulting

9:20 AM

Soft Magnetic Fe-Co-Cu Supersaturated Solid Solutions by Severe Plastic **Deformation**: *Martin Stückler*¹; Heinz Krenn²; Lukas Weissitsch¹; Stefan Wurster¹; Andrea Bachmaier¹; ¹Erich Schmid Institute of Materials Science, Austrian Academy



of Sciences; ²Institute of Physics, University of Graz

9:40 AM Accurate Modelling of Soft Magnetic Materials for Power Applications Using Finite Element Methods: Alex Leary¹; Byron Beddingfield²; Randy Bowman¹; ¹Nasa Glenn Research Center; ²North Carolina State University

10:00 AM

Regression Modelling of the High-frequency Inductors Used for Power Electronic Applications: Sanket Parashar¹; *Richard Beddingfield*; Subhashish Bhattacharya¹; ¹North Carolina State University

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Functional Materials for Energy II

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Wednesday AM March 17, 2021

Session Chairs: Paul Ohodnicki, University of Pittsburgh; Christian Faria, Worcester Polytechnic Institute



Advances in Surface Engineering III — Session I

8:30 AM

Integrated Mo_{1-x}Co_xS₂/Carbon Nanotubes for Water Splitting Applications: Lee *Kendall*¹; Amir Chamaani¹; Stephen McDonnell¹; Giovanni Zangari¹; ¹University of Virginia

8:50 AM

Heterogeneous Metal/Oxide Nanostructure Integration for Catalytic Chemical Transformation: from HCs Oxidation, CO2 Conversion, to H2 Production: Pu-Xian *Gao*¹; ¹University of Connecticut

9:10 AM

High-efficiency High Power Density Direct Carbon Fuel Cell: Christian Faria¹; Jun Lu¹; Adam Powell¹; Boyd Davis²; Yu Zhong¹; Uday Pal³; ¹Worcester Polytechnic Institute; ²Kingston Process Metallurgy; ³Boston University

9:40 AM

Magnesium as a Zero- or Negative-Emissions Fuel for Shipping and Aerospace: Hongyi Sun¹; Yi Jie Wu¹; Jake Scarponi¹; Adam Powell¹; Jagannath Jayachandran¹; ¹Worcester Polytechnic Institute

10:00 AM

Metal Dichalcogenide Based Planner Thermoelectric Generator for Efficient Waste Heat Harvesting: Sangram Pradhan¹; Gilbert Kogo¹; Messaoud Bahoura¹; ¹Norfolk State University

MATERIALS PROCESSING



MOBILE-FRIEND



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee

Program Organizers: Tushar Borkar, Cleveland State University; Arif Mubarok, PPG; Rajeev Gupta, North Carolina State University; Sandip Harimkar, Oklahoma State University; Bharat Jasthi, South Dakota School of Mines & Tech

Wednesday AM March 17, 2021

Session Chairs: Bharat Jasthi, South Dakota School of Mines & Tech; Tushar Borkar, Cleveland State University

8:30 AM

Surface Modification by In-situ Grown VC Reinforced Composite Layer on Steel Substrate Using TIG Arcing Process: Nilesh Kumar¹; Prakriti Ghosh¹; Sourav Das¹; ¹Indian Institute of Technology Roorkee

8:50 AM

Effect of Potassium Hydroxide (KOH) Additives on Corrosion Behavior of Coatings Formed by Plasma Electrolytic Oxidation (PEO) Method on the Titanium Substrate: *Navid Attarzadeh*¹; Maryam Molaei²; Kazem Babaei²; Arash Fattah-alhosseini²; ¹University of Texas at El Paso; ²Bu-Ali Sina University

9:10 AM

Electroplated Powder to Improve Particle Adhesion in Cold Spray Applications: *Gwendolyn Bracker*¹; Elizabeth Hodges¹; Madeline Scott¹; V. Champagne²; Robert Hyers²; ¹University of Massachusetts; ²Cold Spray Innovations International

TMS

MATERIALS DESIGN

Advances in Titanium Technology – Invited Presentations

Sponsored by: TMS Structural Materials Division, TMS: Titanium Committee

Program Organizers: Don Li, Howmet Engineered Products; Yufeng Zheng, University of Nevada-Reno ; Peeyush Nandwana, Oak Ridge National Laboratory; Matthew Dunstan, US Army Research Laboratory

Wednesday AM March 17, 2021

Session Chair: Don Li, Howmet Engineered Products

8:30 AM Invited Titanium Mill Product Yield Enhancement via Electrochemical Conditioning: Kurt Faller¹; ¹MetCon

8:50 AM Invited **Optimizing Microstructure and Properties of Additively Manufactured Titanium** Alloys Using Alloying and Post-AM Heat-treatment: Brian Welk¹; Nevin Taylor¹; Gopal Viswanathan¹; *Hamish Fraser*¹; ¹Ohio State University

9:10 AM Invited

Multiscale Characterization of Titanium Alloy Microstructures and Links to **Processing and Properties**: *Amy Clarke*¹; Benjamin Ellyson¹; Alec Saville¹; Jonah Klemm-Toole¹; Behnam Aminahmadi¹; Jake Benzing²; Adam Creuziger²; Sven Vogel³; Kamel Fezzaa⁴; Wayne Chen⁵; Adam Pilchak⁶; ¹Colorado School of Mines; ²National Institute of Standards and Technology; ³Los Alamos National Laboratory;



⁴Advanced Photon Source, Argonne National Laboratory; ⁵Purdue University; ⁶Air Force Research Laboratory

9:30 AM

Atom Probe Tomographic Study of Precursor Metastable Phases and Their Influence on a Precipitation in the Metastable B-titanium Alloy, Ti-5Al-5Mo-5V-3Cr: Stoichko Antonov¹; Yufeng Zheng²; Hamish Fraser³; Baptiste Gault¹; ¹Max Planck Insitut fur Eisenforschung GmbH; ²University of Nevada, Reno; ³The Ohio State University

9:50 AM

An In-situ Deformation Micro-mechanisms Study of a Ti-Al-V-Fe (a+B) Alloy: Shaolou Wei¹; Gaoming Zhu¹; Cem Tasan¹; ¹Massachusetts Institute of Technology

10:10 AM

Enhanced Work-hardening from Oxygen-stabilized Omega Precipitation in Aged Metastable Beta Ti Alloys: Kathleen Chou¹; Emmanuelle Marquis¹; ¹University of Michigan

MATERIALS DESIGN

AI/Data informatics: Design of Structural Materials — AI/ML for Integrating **Experiments and Simulations; Steels**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Jennifer Carter, Case Western Reserve University; Amit Verma, Carnegie Mellon University; Natasha Vermaak, Lehigh University; Jonathan Zimmerman, Sandia National Laboratories; Darren Pagan, Pennsylvania State University; Chris Haines, Ccdc Army Research Laboratory; Judith Brown, Sandia National Laboratories

Wednesday AM March 17, 2021

8:30 AM Invited A Physics-informed Bayesian Experimental Autonomous Researcher for **Structural Design**: *Keith Brown*¹; ¹Boston University

8:50 AM Solving Inverse Problems for Process-structure Linkages Using Asynchronous **Parallel Bayesian Optimization**: Anh Tran¹; Tim Wildey¹; ¹Sandia National Laboratories

9:10 AM

Model Reification with Batch Bayesian Optimization: *Richard Couperthwaite*¹; Danial Khatamsaz¹; Abhilash Molkeri¹; Douglas Allaire¹; Ankit Srivastava¹; Raymundo Arroyave¹; ¹Texas A&M University

9:30 AM Invited



ONTENTS

Q

WEDNESDAY AM

Structural Response Statistics of Deformed Polycrystals Leading to Rare Events: *Curt Bronkhorst*¹; Peter Marcy²; Hansohl Cho³; Scott Vander Wiel²; Satyapriya Gupta¹; Veronica Anghel²; George Gray²; ¹University of Wisconsin, Madison; ²Los Alamos National Laboratory; ³Korea Advanced Institute of Science and Technology

10:00 AM Invited

Data-driven Approaches for Automated Analysis of Non-metallic Inclusions that Form during Steel Processing: Mohammad Abdulsalam¹; Nan Gao¹; Elizabeth Holm¹; *Bryan Webler*¹; ¹Carnegie Mellon University

10:30 AM

Incorporating Historical Data & Past Analyses for Improved Tensile Property **Prediction of 9% Cr Steel**: *Madison Wenzlick*¹; Ram Devanathan²; Osman Mamun²; Kelly Rose³; Jeffrey Hawk³; ¹Leidos Research Support Team for the National Energy Technology Laboratory; ²Pacific Northwest National Laboratory; ³National Energy Technology Laboratory

MATERIALS DESIGN

AI/Data informatics: Tools for Accelerated Design of High-temperature Alloys - Uncertainty Quantification, AI Tools, and Environmental Degradation

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Michael Titus, Purdue University; Pinar Acar, Virginia Tech; Andrew Detor, GE Research; James Saal, Citrine Informatics; Dongwon Shin, Oak Ridge National Laboratory

Wednesday AM March 17, 2021

TMS WEBSITE

8:30 AM Invited Domain and Uncertainty Quantification in Machine Learning Models of Alloy **Properties**: Dane Morgan¹; Ryan Jacobs¹; Benjamin Blaiszik²; ¹University of Wisconsin-Madison; ²University of Chicago

9:00 AM

Domain Knowledge-informed, Process-mapping AI Graph for Designing Fe**based Alloys**: *Vyacheslav Romanov*¹; ¹National Energy Technology Laboratory

9:20 AM Invited

Toward High Throughput Design and Development of Multi-principal Element Alloys for Corrosion and Oxidation Resistance (MPEAs): Mitra Taheri¹; Todd Hufnagel¹; Chris Wolverton²; James Rondinelli²; Jason Hattrick-Simpers³; Brian DeCost³; Elizabeth Opila⁴; John Scully⁴; Jean-Philippe Couzinie⁵; Nick Birbilis⁶; ¹Johns Hopkins University; ²Northwestern University; ³NIST; ⁴University of Virginia; ⁵University Paris-Est Créteil (UPEC); ⁶Australian National University

9:50 AM

Advanced Data SCiENce Toolkit for Non-data Scientists (ASCENDS)

- A Case Study of the Oxidation Kinetics of NiCr-based Alloys: Jian Peng¹; Rishi Pillai¹; Marie Romedenne¹; Sangkeun Lee¹; Govindarajan Muralidharan¹; Bruce Pint¹; J. Allen Haynes¹; Dongwon Shin¹; ¹Oak Ridge National Laboratory

10:10 AM

Expanding Materials Selection via Transfer Learning for High-temperature Oxide Selection: Zachary Mcclure¹; Alejandro Strachan¹; ¹Purdue University



MOBILE-FRIENDL

10:30 AM Invited OptimalDesignofHigh-temperature,Oxidation-resistantComplexConcentrated **Alloys**: *Alejandro Strachan*¹; ¹Purdue University

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering — Models and Algorithms for Study Microstructures and Mechanical Properties of Materials

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Wednesday AM March 17, 2021

Session Chair: Garritt Tucker. Colorado School of Mines

8:30 AM

Mechanistic Modeling of Point Diffusion in Polycrystals to Capture Different **Diffusion-deformation Mechanisms**: *Aritra Chakraborty*¹; Veerappan Prithivirajan¹; Nathan Beets¹; Arul Kumar Mariyappan¹; Ricardo Lebensohn¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory



Aluminum Alloys, Processing and Characterization — Microstructure Evolution

8:50 AM

Quantitative Phase-field Model for Void Nucleation and Growth Under Ion Irradiation: Rayaprolu Sreekar Annadanam¹; Anter El-Azab¹; ¹Purdue University

9:10 AM

Low Dimensional Polynomial Chaos Expansion Performance at Assessing Uncertainty in Creep Life Prediction of Grade 91 Steel: *Timothy Truster*¹; Amirfarzad Behnam¹; Varun Gupta²; Ramakrishna Tipireddy²; ¹University of Tennessee; ²Pacific Northwest National Laboratory

9:30 AM

Full-field Stress Computation from Measured Deformation Fields: A Hyperbolic **Formulation**: *Benjamin Cameron*¹; Cem Tasan¹; ¹Massachusetts Institute of Technology

9:50 AM

A Simulation Survey of Recrystallization Behavior in Al-xSi Microstructures **Under Shear Loading Conditions**: *William Frazier*¹; Bharat Gwalani¹; Lei Li¹; Ayoub Soulami¹; Arun Devaraj¹; Petr Sushko¹; ¹Pacific Northwest National Laboratory

10:10 AM

Predicting Mechanical Property Parameters from Load-displacement Curve of Nanoindentation Test by Using Machine Learning Model: Jinmyoung Jeon¹; Jungwook Cho¹; Kyojun Hwang¹; ¹GIFT, POSTECH

LIGHT METALS

CONTENTS

TABLE

P



and Characterization

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Dimitry Sediako, University of British Columbia

Wednesday AM March 17, 2021

Session Chair: Izabela Szlufarska, University of Wisconsin-Madison

8:30 AM Invited Microstructure Evolution of an Al-Fe-Ni Alloy with Zr and Sc Additions Upon Different Cooling Rates during Solidification for Improving the Mechanical and Electrical Conductivity Properties: Suwaree Chankitmunkong¹; Dmitry Eskin²; *Chaowalit Limmaneevichitr*¹; ¹King Mongkut's University of Technology Thonburi; ²Brunel University London

8:50 AM

Microstructure and Mechanical Properties of a Precipitation-hardened Al-Mn-Zr-**Er Alloy**: *Amir Farkoosh*¹; David Seidman¹; David Dunand¹; ¹Northwestern University

9:10 AM

Characterization of the Microstructure of Al-Mg Alloy Matrix Syntactic Foam by Three-dimensional Analysis: Jeki Jung¹; Su-Hyeon Kim¹; Won-Kyoung Kim¹; Cha-Yong Lim¹; Yong Ho Park²; ¹Korea Institute of Materials Science; ²Pusan National University/Department of Materials Science and Engineering

9:30 AM

Thermal Analysis of the Solidification Behavior of AA7075 Containing Nanoparticles: *Maximilian Sokoluk*¹; Igor De Rosa¹; Shuaihang Pan¹; Xiaochun Li¹;

¹University of California Los Angeles

9:50 AM

Microstructural Evolution of Ultra-fine Grained (UFGs) Aluminum in Tribological **Contacts**: *Shuguang Wei*¹; Chaiyapat Tangpatjaroen¹; Hongliang Zhang¹; Izabela Szlufarska¹; ¹University of Wisconsin Madison

10:10 AM **Microchemistry Evolution for 8xxx Alloys by Homogenization**: Erik Santora¹; Roland Morak¹; ¹Amag

10:30 AM Question and Answer Period Dr. Dimitry Sediako

BIOMATERIALS

Biological Materials Science – Biological Materials Science I

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Biomaterials Committee**

Program Organizers: David Restrepo, University of Texas at San Antonio; Steven Naleway, University of Utah; Jing Du, Pennsylvania State University; Ning Zhang, University of Alabama

Wednesday AM March 17, 2021

Session Chairs: Steven Naleway, The University of Utah; David Restrepo, The University of Texas at San Antonio



MOBILE-FRIEND

8:30 AM Invited

Understanding the Role of Ridged Geometries in the Telson of the Mantis Shrimp: Adwait Trikanad¹; Wei Huang²; Jesus Rivera³; David Kisailus²; *Pablo Zavattieri*¹; ¹PurdueUniversity;²UniversityofCalifornia,Irvine;³UniversityofCalifornia,Riverside

9:00 AM Invited

Bioinspired Design of Fracture Resistant Layer-by-Layer Composite Structure: *Xinrui Niu*¹; ¹ City University of Hong Kong

9:30 AM

Assessing the Role of Loading Direction on the Compressive Response and Deformation Mechanism in Bioinspired Multilayered Composites: Sashanka *Akurati*¹; Justine Marin¹; Bharath Gundrati¹; Dipankar Ghosh¹; ¹Old Dominion University

9:50 AM Invited Bamboo Fibre-reinforced Mycelium Composites for Sustainable Structures: Hortense Le Ferrand¹; ¹Nanyang Technological University

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII — Structures and Characterization



Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Wednesday AM March 17, 2021

Session Chairs: Robert Maass, Federal Institute of Materials Testing and Research; Joerg Loeffler, ETH Zurich

8:30 AM Invited Ultrafast-calorimetry Experiments to Study Multistep Crystallization and Melting Pathways in Metals: *Joerg Loeffler*¹; ¹ETH Zurich

8:55 AM Invited

Tracing Structural Dynamics in Metallic Glasses during Cryogenic Cycling: Amlan Das¹; Eric Dufresne²; *Robert Maass*³; ¹University of Illinois at Urbana-Champaign; ²Argonne National Laboratory; ³Federal Institute for Materials Research and Testing (BAM)

9:20 AM

The Secondary Phase of Bulk Metallic Glass: *Sydney Corona*¹; Seola Lee¹; Celia Chari¹; Jong Hyun Na²; Konrad Samwer³; William Johnson¹; ¹California Institute of Technology; ²Glassimetal Technologies; ³University of Göttingen

9:40 AM

Fragility, Medium Range Order and Boson Peak in Liquids: *Chae Woo Ryu*¹; Takeshi Egami¹; ¹University of Tennessee

10:00 AM

Non-destructive Probing of Internal Damage Processes in a Metallic Glass: *Amlan Das*¹; Robert Maass²; ¹University of Illinois; ²Federal Institute for Materials Research and Testing

LIGHT METALS

Cast Shop Technology — Metal Cleanliness

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Samuel Wagstaff, Oculatus

Wednesday AM March 17, 2021

Session Chairs: Gerd-Ulrich Gruen, Hydro; Kumar Sundaram, Novelis

8:30 AM

Automated Metal Cleanliness Analyzer (AMCA) – An Alternative Assessment of Metal Cleanliness in Aluminum Melts: *Hannes Zedel*¹; Robert Fritzsch¹; Ragnhild Aune¹; Shahid Akhtar²; ¹NTNU; ²Norsk Hydro

8:50 AM

Overview of the Possibilities and Limitations of the Characterization of Ceramic

Foam Filters for Metal Melt Filtration: *Claudia Voigt*¹; Jana Hubálková¹; Are Bergin²; Robert Fritzsch²; Ragnhild Aune²; Christos G. Aneziris¹; ¹Institute of Ceramic, Glass

MOBILE-FRIEND

and Construction Materials; ²Norwegian University of Science and Technology

9:10 AM

Compression Testing of Ceramic Foam Filters (CFFs) Submerged in Aluminium at Operating Temperature: Are Bergin¹; Robert Fritzsch²; Shahid Akhtar³; Lars Arnberg²; Ragnhild E. Aune²; ¹Norwegian University of Science and Technology & Hydro Aluminium AS; ²Norwegian University of Science and Technology; ³Hydro Aluminium AS

9:30 AM

The Effect of Grain Refiner on Aluminium Filtration: Sarina Bao¹; Jiawei Yang²; Shahid Akhtar³; Stig Tjøtta³; Ulf Tundal³; Tanja Pettersen⁴; Yanjun Li²; ¹SINTEF Materials & Chemistry; ²Norwegian University of Science and Technology; ³Norsk Hydro; ⁴SINTEF Manufacturing

9:50 AM

Next-generation Electrical Preheating System for Filter Boxes: Jochen Schnelle¹; Markus Byczek¹; ¹Drache Umwelttechnik GmbH

10:10 AM

Reduction of Impurity Elements by Applying Electromagnetic Stirring in Fractional Crystallization: Yuichiro Murakami¹; Naoki Omura¹; ¹National Institute of Advanced Industrial Science and Technology

10:30 AM

NatureAlu: Manufacturing High Purity Aluminum from the Concept Idea to the **Production Plant**: Jean Francois Desmeules¹; *Denis Mazerolle*²; ¹Dynamic Concept; ²NatureAlu

NUCLEAR MATERIALS

Ceramic Materials for Nuclear Energy Research and Applications — High **Burnup Oxide Fuels**

Sponsored by: TMS Extraction and Processing Division, TMS Structural Materials Division, TMS Light Metals Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Committee, TMS: Nuclear Materials Committee

Program Organizers: Xian-Ming Bai, Virginia Polytechnic Institute and State University; Yongfeng Zhang, University of Wisconsin-Madison; Larry Aagesen, Idaho National Laboratory; Vincenzo Rondinella, Jrc-Ec

Wednesday AM March 17, 2021

Session Chairs: Miaomiao Jin, Idaho National Laboratory; Karim Ahmed, Texas A&M University

8:30 AM Invited Modeling of Pressure-driven Inter-granular Fracture in High Burnup Structure UO2 during LOCA Using A Phase-field Approach: Wen Jiang¹; Larry Aagesen¹; Kyle Gamble¹; ¹Idaho National Laboratory

9:00 AM

Multiscale Modeling of High Burn-up Structure (HBS) Formation and Evolution in UO2: *Karim Ahmed*¹; Mohammed Abdoelatef¹; Sudipta Biswas²; Larry Aagesen²;

David Andersson³; ¹Texas A&M University; ²INL; ³LANL

- TMS WEBSITE

9:20 AM

A Thermo-mechanical Coupled Phase Field Dynamic Fracture Model and Its Application in UO2: Shuaifang Zhang¹; Wen Jiang²; Michael Tonks¹; ¹University of Florida; ²Idaho National Laboratory

9:40 AM Invited Phase-field Modeling of Bubble Growth During High Burn-up Structure Formation in UO2: Sudipta Biswas¹; Andrea Jokisaari¹; Larry Aagesen¹; ¹Idaho National Laboratory

10:10 AM Invited Electron Microscopy Characterization of the Fuel-cladding Interaction in Annular **Fast Reactor MOX**: *Fabiola Cappia*¹; Alex Winston¹; Brandon Miller¹; Jeffery Aguiar¹; Boopathy Kombaiah¹; Fei Teng¹; Daniel Murray¹; Jason Harp¹; ¹Idaho National Laboratory

10:40 AM

Microstructural and Fission Products Analysis from Irradiated UO2 Fuel Using Atom Probe Tomography: *Mukesh Bachhav*¹; Lingfeng He¹; Brandon Miller¹; Xiang Liu¹; Fabiola Cappia¹; Jian Gan¹; ¹Idaho National Laboratory

CHARACTERIZATION

Characterization of Materials through High Resolution Imaging — High **Resolution Characterization of Materials with Coherent Diffraction Imaging**

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee



WEDNESDAY AM

Program Organizers: Richard Sandberg, Brigham Young University; Ross Harder, Argonne National Laboratory; Xianghui Xiao, Brookhaven National Laboratory; Brian Abbey, La Trobe University; Saryu Fensin, Los Alamos National Laboratory; Ana Diaz, Paul Scherrer Institut; Mathew Cherukara, Argonne National Laboratory

Wednesday AM March 17, 2021

Session Chair: Ana Diaz, Paul Scherrer Institute

8:30 AM Invited Investigating the Early Life on Earth with Nanoscale X-ray Coherent Imaging: Lara *Maldanis*¹; Douglas Galante²; ¹Université Grenoble Alpes; ²Brazilian Synchrotron Light Laboratory

9:00 AM

Confocal Bragg Ptychography for 3D Mapping of Bulk Specimens: Henning Friis Poulsen¹; ¹DTU

9:20 AM

Improve Phase Retrieval Performance in Bragg CDI by Simultaneous **Reconstruction of Multiple Diffraction Peaks**: Yuan Gao¹; Garth Williams¹; ¹Brookhaven National Laboratory

9:40 AM

Near-surface Optical Characterisation of Ion Implantation in Titanium Oxide Thin **Films**: Eugeniu Balaur¹; *Brian Abbey*¹; ¹La Trobe University

10:00 AM Invited

ID01 in Light of the ESRF-EBS: *Steven Leake*¹; Peter Boesecke¹; Tobias Schulli¹;

TMS

¹ESRF - The European Synchrotron

10:30 AM

Retrieving the Full 3D Strain Tensor for Nanoscale Materials Science Applications at 34-ID-C: Anastasios Pateras¹; Ross Harder²; Wonsuk Cha²; Jonathan Gigax¹; Jon Baldwin¹; Jon Tischler²; Ruxing Xu²; Wenjun Liu²; Mark Erdmann²; Robert Kalt²; *Richard Sandberg*³; Saryu Fensin¹; Reeju Pokharel¹; ¹Los Alamos National Laboratory; ²Argonne National Laboratory; ³Bringham Young University

10:50 AM

Multi-peak Phase Retrieval for Coherent X-ray Diffraction Imaging at High **Energies**: *Matthew Wilkin*¹; Anthony Rollett¹; ¹Carnegie Mellon University

11:10 AM Invited

X-ray Imaging of Three-dimensional Magnetic Systems and Their Dynamics: *Claire Donnelly*¹; ¹University of Cambridge

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Characterization of **Mechanical Properties**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos



National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

Wednesday AM March 17, 2021

Session Chairs: Bowen Li, Michigan Technological University; Shadia Ikhmayies, Al Isra University

8:30 AM Effect of Specimen Dimension on Plasticity Behaviour Below Submillimetre Scale: Arijit Lodh¹; Gustavo Castelluccio¹; ¹Cranfield University

8:50 AM

Significant Disparity of Non-basal Dislocation Activities in Hot-rolled Mg and AZ31 Alloy Under Tension: Dexin Zhao¹; Xiaolong Ma¹; Abhinav Srivastavaa¹; Griffin Turner¹; Ibrahim Karaman¹; Kelvin Xie¹; ¹Texas A&M University

9:10 AM

Analysis of Wear Issues in the Rotary Shear Biomass Comminution System: *Kyungjun Lee*¹; Lianshan Lin²; Dave Lanning³; Ercan Cakmak²; James R. Keiser²; Jun Qu²; ¹11612 Lanesborough Way; ²ORNL; ³Forest concepts

9:30 AM

Characterization of Solidification Structure Morphology in High-carbon Steel Billet by Fractal Dimension: Jianghai Cao¹; Zibing Hou¹; Zhiqiang Peng¹; Dongwei Guo¹; Ping Tang¹; ¹Chongqing University

9:50 AM

Dislocation Creep at Low Stresses and High Temperature: Harper-Dorn Creep **Revisited**: *Shobhit Singh*¹; Michael Kassner²; Praveen Kumar¹; ¹Indian Institute of

Science, Bangalore; ²University of Southern California

WEBSITE TMS

The Study of Structure-mechanical Properties Relationship in Different Crosslinked SU-8 Thermoset Polymers: *Prakash Sarkar*¹; Prita Pant¹; Hemant Nanavati¹; ¹Indian Institute of Technology Bombay

NUCLEAR MATERIALS

10:10 AM

Composite Materials for Nuclear Applications — Tungsten

Sponsored by: TMS Structural Materials Division, TMS: Composite Materials Committee, TMS: Nuclear Materials Committee

Program Organizers: Anne Campbell, Oak Ridge National Laboratory; Dong Liu, University of Bristol; Rick Ubic, Boise State University; Lauren Garrison, Oak Ridge National Laboratory; Peng Xu, Idaho National Laboratory; Johann (Hans) **Riesch, Max Planck Institute for Plasma Physics**

Wednesday AM March 17, 2021

Session Chairs: Lauren Garrison, Oak Ridge National Laboratory; Johann Riesch, Max Planck Institute for Plasma Physics

8:30 AM Invited Tungsten-based High and Medium Entropy Alloys and Composites for Nuclear Applications: Owais Waseem¹; *Ho Jin Ryu*²; ¹MIT PSFC; ²KAIST, Korea

9:00 AM Invited

SINEI

0



WEDNESDAY AM

Tungsten Fibre-reinforced Copper – A High-Conductivity, High-Strength **Composite Material for Plasma-facing Component Applications**: Alexander von *Müller*¹; Bernd Böswirth¹; Henri Greuner¹; Rudolf Neu¹; Udo Siefken²; Eliseo Visca³; Jeong-Ha You¹; ¹Max-Planck-Institut für Plasmaphysik; ²Louis Renner GmbH; ³ENEA Frascati

9:30 AM Invited

W₂C-reinforced Tungsten: A Promising Candidate for DEMO Divertor Material: Petra Jenus¹; *Aljaz Ivekovic*¹; Matej Kocen¹; Anze Abram¹; Andreja Sestan¹; Andrei Galatanu²; Magdalena Galatanu²; Sandra Tarancón³; Elena Tejado³; Jose Ygnacio Pastor³; Marius Wirtz⁴; Gerald Pintsuk⁵; Sasa Novak¹; ¹Jožef Stefan Institute; ²National Institute of Materials Physics; ³Universidad Politécnica de Madrid; ⁴Institute for Energy and Climate Reseach, Forschungszentrum Juelich GmbH, ; ⁵Institute for Energy and Climate Reseach, Forschungszentrum Juelich GmbH,

10:00 AM

Solving the Brittleness Problem of Tungsten - Tungsten Fibre-reinforced Tungsten Composites: Johann Riesch¹; Jan Coenen²; Bailey Curzadd¹; Maximilian Fuhr¹; Lauren Garisson³; Hanns Gietl³; Henri Greuner¹; Till Höschen¹; Yiran Mao²; Wolfgang Pantleon⁴; Leonard Raumann²; Daniel Schwalenberg²; Thomas Schwarz-Selinger¹; Dmitry Terentyev⁵; Rudolf Neu¹; ¹Max Planck Institute für Plasma Physics; ²Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC); ³Oak Ridge National Laboratory; ⁴Technical University of Denmark; ⁵Belgian Nuclear Research

10:20 AM

Opportunities for Nanostructured Tungsten Alloys in Composite Fusion Materials: Jason Trelewicz¹; Nicholas Olynik¹; Wenbo Wang¹; David Sprouster¹; Chad Parish²; ¹Stony Brook University; ²Oak Ridge National Laboratory

10:40 AM

Conformal Tungsten Coatings for Cermet Nuclear Fuel Elements: Jonathan Johnson¹; Ryan Wilkerson²; Stephen DiPietro³; Scott O'Dell⁴; Gregory Thompson¹;

MOBILE-FRIEND

¹University of Alabama; ²NASA Marshall Space Flight Center; ³Exothermics Inc; ⁴Plasma Processes LLC

11:00 AM Coupled Primary and Secondary Recrystallization in Single Tungsten Fiberreinforced Tungsten Composites: Umberto Ciucani¹; Lea Haus¹; Maximilian Fuhr²; Hanns Gietl³; Johann Riesch²; *Wolfgang Pantleon*¹; ¹Technical University of Denmark; ²Max-Planck-Institute for Plasma Physics; ³Oak Ridge National Laboratory

ADDITIVE TECHNOLOGIES

Computational Techniques for Multi-Scale Modeling in Advanced Manufacturing — Multiscale Computational Techniques

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Extraction and Processing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, University of Alabama; Mei Li, Ford Motor Company; Alexandra Anderson, Gopher Resource; Srujan Rokkam, Advanced Cooling Technologies Inc

March 17, 2021 Wednesday AM

Session Chair: Adrian Sabau, Oak Ridge National Laboratory



WEDNESDAY AM

TABLE

Q

NTENTS

8:30 AM

Machine-learning Informed Design of High-strength Gradient Metals for Additive Manufacturing: S. Mohadeseh Taheri-Mousavi¹; A. John Hart¹; ¹MIT

8:55 AM

A Hybrid Approach to Connecting a Low Fidelity Model to a High Fidelity Model for Efficient and Accurate Prediction of Thermal History of Large Domains in Additive Manufacturing: Christopher Katinas¹; Corbin Grohol¹; Yung Shin¹; ¹Purdue University

9:20 AM Invited

Predicting Mechanical Performance in Additive Manufacturing Components Using Deep Learning: *Kyle Johnson*¹; John Emery¹; Demitri Maestas¹; Matthew Smith¹; Carianne Martinez¹; Mircea Grigoriu²; ¹Sandia National Laboratories; ²Cornell University

10:00 AM

Smoothed Particle Hydrodynamics based approach for 3D Modeling of Linear Friction Welding Process: Srujan Rokkam¹; Quang Truong¹; ¹Advanced Cooling Technologies Inc

10:25 AM

Synchrotron Calibrated Lagrangian Particle Tracking of Melt-pool Ejections during Laser Powder Bed Fusion: Samuel Clark¹; Gongyuan Zeng²; Juergen Jakumeit²; Chu Lun Alex Leung¹; Yunhui Chen¹; Sebastian Marussi¹; Lorna Sinclair¹; Margie Olbinado³; Alexander Rack⁴; Peter Lee¹; ¹University College London; ²Access e.V.; ³Paul Scherrer Institute; ⁴European Synchrotron Radiation Facility

PHYSICAL METALLURGY

TMS

Computational Thermodynamics and Kinetics — Solidification, Additive

Manufacturing / Ordering, Coarsening and Patterning

WEDNESDAY AM

NTENTS **P**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

March 17, 2021 Wednesday AM

Session Chairs: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Vahid Attari, Texas A&M University; Eva Zarkadoula, Oak Ridge National Laboratory; Laurent Béland, Queen's University

8:30 AM Invited Influence of Interphase Boundary Anisotropy on the Formation of Lamellar Eutectic Solidification Patterns: Mathis Plapp¹; Supriyo Ghosh²; Sabine Bottin-Rousseau³; Silvère Akamatsu³; ¹Ecole Polytechnique, CNRS; ²Los Alamos National Laboratory; ³Sorbonne Université, CNRS

9:00 AM

Thermokinetics and Associated Microstructural Evolution of Laser Powder Bed **Fused Additively Manufactured Ti6Al4V**: *Mangesh Pantawane*¹; Narendra Dahotre¹; ¹University of North Texas

9:20 AM Invited



Inhomogeneous Free Energies Beyond the Cahn-Hilliard Model: Interface Anisotropy and Equilibrium Patterning: *Pascal Bellon*¹; Qun Li¹; Robert Averback¹; ¹University of Illinois at Urbana-Champaign

9:50 AM

Topological Transitions during Coarsening in Nanoporous Metals: *Kate Elder*¹; W. Beck Andrews²; Markus Ziehmer³; Alexander Chadwick¹; Erica Lilleodden³; Katsuyo Thornton²; Peter Voorhees¹; ¹Northwestern University; ²University of Michigan; ³Helmholtz-Zentrum Geesthacht

PHYSICAL METALLURGY

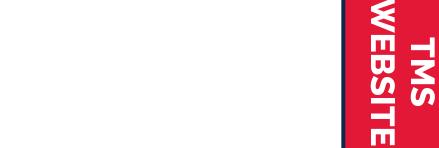
Defect and Phase Transformation Pathway Engineering for Desired Microstructures — Experiment and Characterization

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Yufeng Zheng, University of Nevada-Reno ; Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Timofey Frolov, Lawrence Livermore National Laboratory; Stoichko Antonov, Max-Planck-Institut für Eisenforschung GmbH; Jessica Krogstad, University of Illinois at Urbana-Champaign; Bin Li, University of Nevada, Reno

March 17, 2021 Wednesday AM

Session Chair: Stoichko Antonov, Max Planck Insitut fur Eisenforschung GmbH



8:30 AM

Grain Boundary Segregation for Thermal Stability in Ternary Nanocrystalline Alloys: *Sebastian Kube*¹; Wenting Xing²; Arvind Kalidindi²; Sungwoo Sohn¹; Amit Datye¹; Dor Amram²; Christopher Schuh²; Jan Schroers¹; ¹Yale University; ²Massachusetts Institute of Technology

8:50 AM

Tuning Fine-scale Alpha Microstructures via Nano-scale Structural and Compositional Non-uniformities in Beta Titanium Alloys: Dian Li¹; Rongpei Shi²; Rajarshi Banerjee³; Yunzhi Wang⁴; Hamish Fraser⁴; *Yufeng Zheng*¹; ¹University of Nevada, Reno; ²Lawrence Livermore National Laboratory; ³University of North Texas; ⁴Ohio State University

9:10 AM

Exploring the Microstructure of Sputtered Nanotwinned Alloys and Its Role in the Study of Dislocation-Twin Interactions: *Francisco Andrade Chávez*¹; Orcun Koray Calebi¹; Ahmed Sameer Khan Mohammed¹; Huseyin Sehitoglu¹; Jessica Krogstad¹; ¹University of Illinois at Urbana-Champaign

9:30 AM

Pseudo-in situ Characterization of Phase Transformation in an Al-Cu-Mn-Zr Alloy Using Atom Probe Tomography: *Bharat Gwalani*¹; Jia Liu¹; Jonathan Poplawsky²; Amit Shyam²; Arun Devaraj¹; ¹Pacific Northwest National Laboratory; ²Oak Ridge National Lab

9:50 AM High-temperature Bulk Dislocation Dynamics in Aluminum: *Leora Dresselhaus-Marais*¹; ¹Lawrence Livermore National Laboratory



WEDNESDAY AM

CONTENTS

TABLE

Q

10:10 AM

Interaction between Martensite Transformation and Ion-induced Damage in Shape Memory Alloys: *Alejandro Hinojos*¹; Daniel Hong¹; Nan Li²; Khalid Hattar³; Peter Anderson¹; Michael Mills¹; ¹The Ohio State University; ²Los Alamos National Labs; ³Sandia National Labs

10:30 AM

Microstructural Evolution of Nanotwinned Al-Zr Alloy with Significant 9R Phase Stabilization: *Nick Richter*¹; Yifan Zhang¹; Ruizhe Su¹; Tongjun Niu¹; Qiang Li¹; Sichuang Xue¹; Haiyan Wang¹; Xinghang Zhang¹; ¹Purdue University

MATERIALS PROCESSING

Deformation Induced Microstructural Modification — Session V: Deformation of Alloys II and Composites

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside ; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

Wednesday AM March 17, 2021

Session Chair: Kester Clarke, Colorado School of Mines

Grain Refinement and Bimodal Distribution of Precipitates in Al 6xxx and 7xxx Alloys during ShAPE (Shear Assisted Processing and Extrusion): Xiaolong Ma¹;

Rajib Kalsar¹; Jens Darsell¹; Miao Song¹; Nicole Overman¹; Keerti Kappagantula¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory

8:50 AM

Influence of Shear Rolling on Microstructure and Properties of Low-density Steels:

*Dean Pierce*¹; Tomas Scuseria¹; Kelcey Garza¹; Amrinder Gill¹; Jerry Arnold¹; Amy Clarke¹; Kester Clarke¹; Ercan Cakmak¹; Artem Trofimov¹; Hsin Wang¹; Govindarajan Muralidharan¹; Tom Muth¹; ¹Oak Ridge National Laboratory

9:10 AM

Investigation of Path Dependent Microstructural Evolution in Cu-Nb System **Processed via Friction Consolidation**: *Mageshwari Komarasamy*¹; Xiao Li¹; Scott Whalen¹; Xiaolong Ma¹; Nathan Canfield¹; Matthew Olszta¹; Tamas Varga¹; Glenn Grant¹; Suveen Mathaudhu²; ¹Pacific Northwest National Laboratory; ²University of California, Riverside and Pacific Northwest National Laboratory

9:30 AM

Low Temperature Superplasticity in Al 5083 Produced by Accumulative Roll **Bonding**: *Brady McBride*¹; Kester Clarke¹; Amy Clakre¹; ¹Colorado School of Mines

9:50 AM

Tailoring the Mechanical Performance in Novel Zn-Ag-Mg Alloy Processed by Cold Plastic Deformation Processes: Maria Watroba¹; Wiktor Bednarczyk¹; Jakub Kawalko¹; Terence G. Langdon²; Piotr Bala¹; ¹AGH University of Science and Technology; ²University of Southampton

10:10 AM

The Unusual Effect of HPT Processing on Microstructure and Mechanical **Properties in Zn-alloys**: *Wiktor Bednarczyk*¹; Maria Watroba¹; Jakub Kawalko¹; Piotr Bala¹; Terence G. Langdon²; ¹AGH University of Science and Technology in Krakow; ²University of Southampton



WEDNESDAY AM

TABLE OF

10:30 AM

Mg-Fe Bonded Interface Using FaST: Hrishikesh Das¹; Tianhao Wang¹; Piyush Upadhyay¹; Bharat Gwalani¹; Xiaolong Ma¹; Dalong Zhang¹; ¹Pacific Northwest National Laboratory

10:50 AM

Harnessing Thermomechanical Processing to Influence Texture in ARB Cu/Nb **Composites**: Justin Cheng¹; Sven Vogel²; Cody Miller²; Ryan Mier²; Carl Osborn²; John Carpenter²; Madhavan Radhakrishnan³; Osman Anderoglu³; Nathan Mara¹; ¹University of Minnesota Twin Cities; ²Los Alamos National Laboratory; ³University of New Mexico

11:10 AM

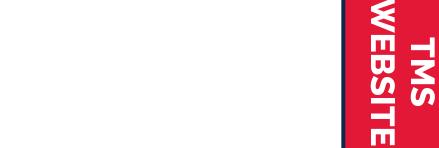
Evolution of Mechanical Properties and Microstructure in Accumulative Roll Bonded FCC/BCC Metallic Composites: *Thomas Nizolek*¹; Daniel Coughlin¹; Cody Miller¹; Nan Li¹; Rodney McCabe¹; John Carpenter¹; ¹Los Alamos National Laboratory

11:30 AM

Analysis of Al 6061 and Mild Steel Joints from Rotary Friction Welding: Nikhil *Gotawala*¹; Amber Shrivastava¹; ¹Indian Institute of Technology Bombay

LIGHT METALS

Electrode Technology for Aluminum Production – Anode Production - Green & Baked Anode Production/Modelling and Performance



Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Derek Santangelo, Hatch

Wednesday AM March 17, 2021

Session Chair: Julien Lauzon-Gauthier, Alcoa Corporation

8:30 AM Start-up of a New "Smart & Green" Anode Plant: Christophe Bouche¹; Xavier Genin¹; Vincent Philippaux¹; Jérôme Morfoise¹; ¹Fives

8:50 AM

The Steps to Optimize and Implement an Anode Stub Hole Cleaning Machine **Modification**: *Valerie Langelier*¹; Derek Santangelo¹; ¹Hatch

9:10 AM **Biocarbon in the Aluminium Industry: A Review**: Samuel Senanu¹; Asbjørn Solheim¹; ¹SINTEF

9:30 AM

Anode to Cathode Electrical Current Modelling for Cell Retrofit Application of **Conductive Nails Technology**: *William Berends*¹; ¹Alucelltech Inc.

9:50 AM

Managing Anode Performance with a Versatile Reactivity Analysis Method: Lorentz Petter Lossius¹; Juraj Chmelar¹; Viktorija Tomkute¹; ¹Hydro Aluminium AS



MOBILE-FRIEND

ELECTRONIC MATERIALS

Electronic Packaging and Interconnections 2021 — Advanced Microelectronic Packaging Materials

Sponsored by: TMS Functional Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

Program Organizers: Mehran Maalekian, Mat-Tech; Christopher Gourlay, Imperial College London; Babak Arfaei, Ford Motor Company; Praveen Kumar, Indian Institute of Science; Sai Vadlamani, Intel Corporation; Kazuhiro Nogita, University of Queensland; David Yan, San Jose State University

Wednesday AM March 17, 2021

Session Chairs: Sai Vadlamani, Intel Corp.; Prithwish Chatterjee, Intel Corp.

8:30 AM Invited Advances in Low Temperature/Low Pressure Ag Sinter Joining and Its Thermal Performance: Katsuaki Suganuma¹; Chuantong Chen¹; Zheng Zhang¹; Aiji Suetake¹; Aya Iwaki¹; Ming Hsieh¹; Naoki Sato¹; ¹Osaka University

8:50 AM

Electric-enhanced Sintering of Copper Interconnects: Tzu-Hao Shen¹; Albert T. Wu¹; ¹National Central University

9:10 AM



9:30 AM

Plasticity and Contact Resistance Behavior in Wirebond Packaging: Allison Osmanson¹; Mohsen Tajedini¹; Hossein Madanipour¹; Yi Ram Kim¹; Choong-Un Kim¹; ¹University of Texas at Arlington

9:50 AM

The Effects of DC, Pulsed DC, and AC Load Conditions on Electromigration Failure Mechanism in Solder Interconnects: *Yi Ram Kim*¹; Hossein Madanipour¹; Allison Osmanson¹; Mohsen Tajedini¹; Choong-Un Kim¹; Patrick Thompson²; Qiao Chen²; ¹University of Texas at Arlington; ²Texas Instruments, Inc.

10:10 AM

Sintered Micro-silver Joints with the Addition of Indium Applied to Power IC Packaging: *Chin-Hao Tsai*¹; Wei-Chen Huang¹; Ly May Chew²; Wolfgang Schmitt²; Hiroshi Nishikawa³; C. Robert Kao¹; ¹National Taiwan University; ²Heraeus Deutschland GmbH & Co. KG; ³Joining and Welding Research Institute, Osaka University

10:30 AM

Low-Temperature and Pressureless Cu-to-Cu Bonding by Electroless Pd Plating Using Microfluidic System: *Po Shao Shih*¹; Zhen De Ma¹; Han Tang Hung¹; Jeng Hau Huang¹; C.Robert Kao¹; ¹National Taiwan University

CORROSION

Environmental Degradation of Additively Manufactured Alloys — High



Temperature Oxidation and Corrosion, High Temperature Alloys

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Additive Manufacturing Committee

Program Organizers: Kinga Unocic, Oak Ridge National Laboratory; Jenifer Locke, Ohio State University; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Xiaoyuan Lou, Auburn University; Brendy Rincon Troconis, University of Texas at San Antonio; Luke Brewer, University of Alabama

Wednesday AM March 17, 2021

Session Chairs: Kinga Unocic, Oak Ridge National Laboratory; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory

8:30 AM Invited High Temperature Air Oxidation Behavior of Ni-based Superalloys Processed by Electron Beam Melting (EBM) and Selective Laser Melting (SLM): Marie Romedenne¹; Rishi Pillai¹; Sebastien Dryepondt¹; ¹ORNL

9:00 AM Invited Effect of High-temperature Oxidation on the Fatigue Properties of Inconel 625 Fabricated by Laser Additive Manufacturing: *Grace De Leon Nope*¹; Juan Alvarado-Orozco²; Guofeng Wang¹; Brian Gleeson¹; ¹University of Pittsburgh; ²CIDESI

9:30 AM Invited

High Temperature Oxidation of Additively Manufactured FeCrAl and Ni-based Alloys: *Mohammad Sattari*¹; Irina Fedorova¹; Alberto Visibile¹; Kerem Gündüz¹; Jan

Froitzheim¹; Krystyna Stiller¹; Mats Halvarsson¹; ¹Chalmers University of Technology

10:00 AM

Microstructural Evolution and Oxidation Behavior of Fe-25Cr-20Ni-1.4Nb-0.2C Steel Fabricated by Laser Powder-bed Fusion: *Kinga Unocic*¹; Marie Romedenne¹; Peeyush Nandwana¹; Sebastien Dryepondt¹; ¹Oak Ridge National Laboratory

10:20 AM Invited

High Temperature Oxidation and Corrosion of LBM and EBM Ni-base Superalloys and Ti Alloys: Daniel Monceau¹; Tom Sanviemvongsak²; Antoine Casadebaigt³; Annabelle Vernouillet⁴; Bruno Macquaire⁵; Jonathan Hugues⁶; Sebastien Doublet⁷; Aurélie Vande Put¹; ¹CIRIMAT Laboratory; ²CIRIMAT Laboratory; Safran Tech; ³CIRIMAT Laboratory; IRT Saint Exupery; ⁴CIRIMAT Laboratory; Air Liquide; ⁵Safran Tech; ⁶IRT Saint Exupery; ⁷Air Liquide

CORROSION

Environmentally Assisted Cracking: Theory and Practice – Innovative Techniques in Corrosion Research

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Wednesday AM March 17, 2021

Session Chairs: Khalid Hattar, Sandia National Lab; Michele Manuel, University of



Florida

8:30 AM Invited Deconvoluting Mechanism in Complex Environments via In-situ Electron **Microscopy**: *Khalid Hattar*¹; ¹Sandia National Laboratories

9:10 AM Invited Elucidation of Corrosion Mechanisms in Light Alloys by In situ X-ray Micro and **Nanotomography**: *Nikhilesh Chawla*¹; ¹Purdue University

9:50 AM Invited Controlling the Corrosion Behavior of Bioresorbable Magnesium Implants: *Michele Manuel*¹; ¹University of Florida

10:30 AM Invited Understanding General Grain Boundaries: The Weak Link for Mechanical and Chemical Degradation: *Jian Luo*¹; ¹University of California, San Diego

11:10 AM Classifying Liquid-solid Metal Interactions: Separation of the Multiple Mechanisms of Liquid Metal Embrittlement: Justin Norkett¹; Cameron Frampton¹; *Victoria Miller*¹; ¹University of Florida

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and Computational Modeling — From Cyclic Plastic Localization and Accumulation to Crack Nucleation and Propagation



Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear, University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara

Wednesday AM March 17, 2021

Session Chair: Jean-Charles Stinville, University of California - Santa Barbara

8:30 AM

Fatigue and Dwell-fatigue Crack Initiation at (OOO1) Twist Boundaries in Ti Alloys: Cyril Lavogiez¹; Jean-Charles Stinville²; Tresa Pollock²; Paraskevas Kontis³; Valéry Valle⁴; Patrick Villechaise¹; *Samuel Hemery*⁵; ¹ISAE-ENSMA; ²University of California Santa Barbara; ³MPIE; ⁴Université de Poitiers; ⁵Institute Prime - Ensma

8:50 AM Multi-scale Analysis of Fatigue Damage in Welded Lean Duplex Stainless Steel Components: *Ayoub Elmoutaouakkil*¹; Anna Fraczkiewicz¹; Alexandre Gay²; Jacques Stolarz¹; ¹Emse; ²e.l.m. Leblanc

9:10 AM Invited





TABL

P

NTENTS

Tracking Crystal-scale Cyclic Plasticity in Inconel 718 Using High Energy X-rays: *Dalton Shadle*¹; Kelly Nygren²; Matthew Miller¹; ¹Cornell University; ²Cornell High Energy Synchrotron Source

9:30 AM

Plastic Localization in Solid Solution and Precipitation Strengthened Inconel 718 and Its Effect on VHCF Properties: *Alice Cervellon*¹; Damien Texier²; Marie Agathe Charpagne¹; Chris Torbet¹; Valéry Valle³; Jean Charles Stinville¹; Tresa Pollock¹; ¹University of California Santa Barbara; ²Institut Clément Ader; ³Institut Pprime

9:50 AM

Microstructural and Mechanical Evolution of Aluminum 7075-T6 during Nonreversible Fatigue Loading: *Joseph Indeck*¹; Gabriel Demeneghi¹; Jason Mayeur¹; Cyril Williams²; Kavan Hazeli¹; ¹The University of Alabama in Huntsville; ²U.S. Army Research Laboratory

10:10 AM

Effect of Microtexture on Minimum Dwell Fatigue Life of Ti-6Al-4V: *Sushant Jha*¹; Daniel Sparkman²; James Larsen²; Reji John²; Adam Pilchak²; ¹University of Dayton Research Institute; ²US Air Force Research Laboratory

10:30 AM

On the Role of Annealing Twin Boundaries in the Cyclic Plastic Strain Localization and the Fatigue Crack Initiation in Equiatomic CrCoNi Medium-entropy Alloy: *Veronika Mazánová*¹; Milan Heczko¹; Connor Slone¹; Ivo Kubena²; Easo George³; Maryam Ghazisaeidi¹; Tomas Kruml²; Jaroslav Polak²; Michael Mills¹; ¹The Ohio State University; ²Institute of Physics of Materials CAS; ³Oak Ridge National Laboratory

10:50 AM Reminder ... A joint session, "Microstructure-based Fatigue Studies on Additive-Manufactured Materials," will be held on Wednesday at 2 p.m. EDT in conjunction with the Additive Manufacturing Fatigue and Fracture V: Processing-

TMS

Structure-Property Investigations and Application to Qualification symposium.



CONTENTS

FABLE OF

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Dissimilar

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St. Petersburg Polytechnic University

Wednesday AM March 17, 2021

8:30 AM Invited Friction Stir Welding of Metal and Carbon Fiber Reinforced Plastic: Hidetoshi *Fujii*¹; Jeong-Won Choi¹; Yoshiaki Morisada¹; Kimiaki Nagatsuka¹; Kazuhiro Nakata¹; ¹Osaka University

8:50 AM

Friction Stir Welding of Metal Matrix Composites to Dissimilar Aluminum Alloys: **Optimization of Weld Quality and Tool Life**

: *Michael Eff*¹; Scott Rose²; Kyung Chung³; Don Hashiguchi³; Drew Shipley¹; Elizabeth Burns²; ¹EWI; ²Boeing; ³Materion

9:10 AM

Dissimilar Joining of ZEK100 and AA6022 for Automotive Application: Hrishikesh

*Das*¹; Piyush Upadhyay¹; Woongjo Choi¹; Shank Kulkarni¹; ¹Pacific Northwest National Laboratory

9:30 AM

Fracture Mechanics Approach to Improve Fatigue Strength of a Dissimilar Metal T-Lap Joint by Friction Stir Welding: Masakazu Okazaki¹; Hao Duong¹; Satoshi Hirano²; ¹Nagaoka University of Technology; ²Hitachi Research Laboratory

9:50 AM

Effect of Diffusion on Intermetallics at Interface during Friction Stir Welding of Stainless Steel and Pure Titanium: Nikhil Gotawala¹; Amber Shrivastava¹; ¹Indian Institute of Technology Bombay

10:10 AM

Microstructural and Mechanical Characterization of Titanium/Steel Joints Produced by Ultrasound Enhanced Friction Stir Welding: Andreas Gester¹; Marco Thomae¹; Guntram Wagner¹; ¹Chemnitz University of Technology

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Melting, Nucleation & Laser **Processing**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Wednesday AM March 17, 2021

Session Chairs: Julien Zollinger, Institut Jean Lamour; Amy Clarke, Colorado School of Mines; Guillaume Boussinot, Access e.V.; Tiberiu Stan, Northwestern University

8:30 AM Invited Melting of Metastable Solid-states in Au-Si Eutectic Alloy: *Güven Kurtuldu*¹; ¹ETH Zürich

9:00 AM Invited Microstructure Evolution during Melting: *Guillaume Boussinot*¹; Mahdi Torabi Rad¹; Markus Apel¹; Alexandre Viardin¹; ¹Access e.V.

9:30 AM Invited ISRO-mediated Nucleation in Fcc Alloys during Rapid Melting and Solidification Processes: Julien Zollinger¹; Ivan Cazic²; Michel Rappaz³; Benoît Appolaire¹; ¹Institut Jean Lamour; ²Institut Jean Lamour / Institut de Soudure; ³EPFL



10:00 AM

Orientation Relationships between Al3Ti and TiB2 due to Nucleation and Pushing/Engulfment: Yi Cui¹; Andrew Horsfield¹; *Christopher Gourlay*¹; ¹Imperial College London

10:20 AM

Model the Initiation of Hot Cracking in Aluminum 6061 during the Processes of Laser Welding: *Guannan Tang*¹; Anthony Rollett¹; ¹Carnegie Mellon University

10:40 AM

Using Composition and Patterning to Induce Solidification Instabilities in Al-Cu Eutectic Thin Films: *Eli Sullivan*¹; John Tomko¹; Jonathan Skelton¹; James Fitz-Gerald¹; Patrick Hopkins¹; Jerrold Floro¹; ¹University of Virginia

SPECIAL TOPICS

Frontiers of Materials Award Symposium: Low-Dimensional Materials and Interfaces for Next Generation Computing — Session II

Program Organizer: Deep Jariwala, University of Pennsylvania

Wednesday AM March 17, 2021

8:30 AM Invited Designing Solid-state Materials from Quantum Dots for Next-generation Electronic Devices: *Cherie Kagan*¹; ¹University of Pennsylvania

9:10 AM Invited

vdW Contacts on 2D Semiconductors: Manish Chhowalla¹; ¹Cambridge University

8:55 AM

9:50 AM Panel Discussion Moderator: Deep Jariwala; Panelists: Mark C. Hersam, Suman Datta, Cherie Kagan, and Manish Chhowalla

NANOSTRUCTURED MATERIALS

Functional Nanomaterials: Functional Low-dimensional Materials (OD, 1D, 2D) Driving Innovations in Electronics, Energy, Sensors, and Environmental Engineering and Science 2021 — Nanomanufacturing & Sensors

Sponsored by: TMS Functional Materials Division, TMS: Nanomaterials Committee

Program Organizers: Jiyoung Chang, University of Utah; Michael Cai Wang, University of South Florida; Sarah Zhong, University of South Florida; Sun Choi, Korea Institute of Science and Technology; Pei Dong, George Mason University

Wednesday AM March 17, 2021

Session Chairs: Jiyoung Chang, University of Utah; Sun Choi, Korea Institute of Science and Technology

8:30 AM Invited In-situ Production of Metal Nanoparticles on Polymer Derived Ceramic Fibers for Catalysis and Sensing: Sajia Afrin¹; Jean Calderon¹; *Lei Zhai*¹; ¹University of Central Florida





Suspended Graphene H2 Sensors With Enhanced Sensitivity Fabricated Using Direct-write Functional Fibers: *Abiral Regmi*¹; Dongwoon Shin¹; Noori Na¹; Jiyoung Chang¹; ¹University of Utah

9:15 AM Invited Laser Digital Patterning for Nickel-based Flexible Electrodes and Its Applications for Electronics and Sensors: *Daeho Lee*¹; ¹Gachon University

9:40 AM Invited Redesigning Batteries via Additive Manufacturing: *Corie Cobb*¹; ¹University of Washington

10:20 AM Invited Ultra-fast Nanomaterial Assembly and R2R Printing for High-performance Skin Sensors: *Ying Zhong*¹; Long Wang²; Rui Kou²; ¹University of South Florida; ²University of California at San Diego

10:45 AM

Transparent and Flexible Nanoelectrodes for Wearable Electronics by Directwriting of PEDOT:PSS-nanofiber: *Dongwoon Shin*¹; Abiral Regmi¹; Jiyoung Chang¹; ¹University of Utah

11:05 AM

Wireless Strain Field Mapping of Metallic Surfaces through THz Time Domain Spectroscopy of Electrostrictive Coating Acting as Passive Sensor: Luis Reig Buades¹; Abhijeet Dhiman¹; Vikas Tomar¹; ¹Purdue University

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for

TMS

Superior Properties — Harmonic Structure, Composites and Films

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

Wednesday AM March 17, 2021

Session Chairs: Kei Ameyama, Ritsumeikan University; Dmytro Orlov, Lund University; Benjamin Guennec, Toyama Prefectural University

8:30 AM

Unique Hall-petch Relation in Harmonic Structure Materials: *Kei Ameyama*¹; ¹Ritsumeikan University

8:50 AM Invited SizeEffectIssueontheFatiqu

Size Effect Issue on the Fatigue Properties of Ti-6Al-4V Designed in Heterogeneous Harmonic Structure: *Benjamin Guennec*¹; Takayuki Ishiguri²; Mie Ota Kawabata³; Shoichi Kikuchi⁴; Akira Ueno³; Kei Ameyama³; ¹Toyama Prefectural University; ²Mitsui High-tec; ³Ritsumeikan University; ⁴Shizuoka University

9:15 AM

Yielding in a Metallic Nanocomposite at the Nanoscale: *Kangpyo So*¹; Myles Stapelberg¹; Yu Ren Zhou¹; Hideki Mori²; Shigenobu Ogata²; Michael Short¹; Ju Li²; Sidney Yip¹; ¹Massachusetts Institute Of Technology; ²College of Industrial Technology



9:35 AM Invited Lattice Defect Development in Harmonic Metals through Atomic Simulations: *Tomotsugu Shimokawa*¹; Tatsuya Hasegawa¹; Tomoaki Niiyama¹; ¹Kanazawa University

10:00 AM Invited

Backstress Development and Strain Partitioning in Harmonic-structure Materials: *Dmytro Orlov*¹; Roman Kulagin²; Yan Beygelzimer³; ¹Lund University; ²Karlsruhe Institute of Technology; ³Donetsk Institute for Physics and Engineering

10:25 AM Invited Outstanding Mechanical Properties in a Harmonic Structure Designed Titanium Due to Preferential Recrystallization: *Bhupendra Sharma*¹; Motoki Miyakoshi¹; Mie Kawabata¹; Kei Ameyama¹; ¹Ritsumeikan University

10:50 AM

High Strength and Tensile Ductility in Bicrystalline Nickel Thin Films with Incoherent Twin Boundaries: Rohit Berlia¹; *Jagannathan Rajagopalan*; ¹Arizona State University

11:10 AM

Effect of Rolling on Fatigue Crack Propagation in Harmonic Structured Commercially Pure Titanium: Yoshikazu Nakai¹; Shoichi Kikuchi²; Kohei Osaki¹; Mie Kawabata³; Kei Ameyama³; ¹Kobe Univ; ²Shizuoka University; ³Ritsumeikan University

11:30 AM

Synthesis and Mechanical Characterization of Metallic Films with Precisely

TMS

Defined Heterogeneous Microstructures: Rohit Berlia¹; *Jagannathan Rajagopalan*;

¹Arizona State University

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Joint Session with Materials for High Temperature Applications: Next Generation Superalloys and **Beyond**

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Wednesday AM March 17, 2021

Session Chairs: Oleg Senkov, Air Force Research Laboratory; Ridwan Sakidja, Missouri State University

8:30 AM Invited **Temperature Dependent Deformation Behavior and Strengthening Mechanisms** in a Two-phase BCC+B2 Refractory High Entropy Alloy: Oleg Senkov¹; Jean-Philippe Couzinie²; Satish Rao¹; Vishal Soni³; Rajarshi Banerjee³; ¹Air Force Research Laboratory; ²Université Paris Est Creteil; ³University of North Texas

MOBILE-FRIEND

8:55 AM Invited

Mechanical Properties of Precipitation Strengthened Refractory High Entropy Alloys at Elevated Temperatures: Stephan Laube¹; Steven Schellert²; Daniel Schliephake¹; Alexander Kauffmann¹; Bronislava Gorr²; Hans-Jürgen Christ²; Martin Heilmaier¹; ¹Karlsruher Institut für Technologie (KIT); ²Universität Siegen

9:20 AM

Transport Properties of Binary and Entropy-stabilized Diborides: Alin Niraula¹; BikashTimalsina¹; Gregory Hilmas²; William Fahrenholtz²; Ridwan Sakidja¹; ¹Missouri state university; ²Missouri university of Science and technology

9:40 AM Invited The Design and Characterization of High Entropy Alloys for High Temperature Applications: *Kevin Garber*¹; Bhaskar Majumdar¹; ¹New Mexico Institute of Mining and Technology

10:05 AM Invited

Unique Microstructural Evolution and Deformation Behavior of HfNbTaTiZr BCC High Entropy Alloy at Elevated Temperatures: Nobuhiro Tsuji¹; Rajeshwar Eleti¹; Atul Chokshi²; Akinobu Shibata³; ¹Kyoto University; ²Indian Institute of Science; ³National Institute for Materials Science (NIMS)

10:30 AM Invited

Design of Corrosion and Irradiation Resistant Compositionally Complex Alloys Using a High-throughput Platform for Applications in Extreme Environments: Adrien Couet¹; Michael Moorehead¹; Michael Niezgoda¹; Phalgun Nelaturu¹; Bonita Goh¹; Yafei Wang¹; Mediha Karatas¹; Chuan Zhang²; Fan Zhang²; Thien Duong³; Santanu Chaudhuri³; Kumar Sridharan¹; Dan Thoma¹; ¹University of Wisconsin-Madison; ²Computherm LLC; ³Argonne National Laboratory

10:55 AM



8:50 AM Invited

Takata²; Kyoko Kawagishi¹; Hideyuki Murakami¹; ¹National Institute for Materials Science / Waseda University; ²National Institute for Materials Science

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling - Structures and Characterization II

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Wednesday AM March 17, 2021

Session Chairs: James Morris, Ames Laboratory; Yang Ren, Argonne National Laboratory

8:30 AM Invited Predicting High Entropy Alloy Behavior: What We Can Learn from Non-empirical **Approaches**: James Morris¹; ¹Ames Laboratory





Role of Local Chemical Order in Orientation Relationship Determination in an AlO.3CoCrFeNi High Entropy Alloys: *Elaf Anber*¹; Daniel Foley¹; Diana Farkas²; Peter Liaw³; Mitra Taheri¹; ¹Johns Hopkins University; ²Virginia Tech; ³The University of Tennessee

9:10 AM

Microstructure and Mechanical Properties of a Dual Phase Transformation Induced Plasticity Fe-Mn-Co-Cr High Entropy Alloy: AFM Monowar Hossain¹; Rajiv Mishra²; Nilesh Kumar¹; ¹University of Alabama Tuscaloosa; ²University of North Texas

MATERIALS PROCESSING

High Temperature Electrochemistry IV – Session IV

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Guy Fredrickson, Idaho National Laboratory

Wednesday AM March 17, 2021

Session Chair: Guy Fredrickson, Idaho National Laboratory

8:30 AM Interaction between Solute Species and Metallic Alloying Elements in Molten **Chloride Systems**: *William Phillips*¹; Ruchi Gakhar¹; ¹Idaho National Laboratory



TENTS

9

9:00 AM Effect of Hydroxide and Oxide Impurities in Electrochemical Processes Using Molten LiCland CaCl,: Mario Alberto Gonzalez¹; Emma Faulkner¹; Michael Simpson¹; ¹University of Utah

MATERIALS DESIGN

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session V

Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

Wednesday AM March 17, 2021

Session Chairs: Greta Lindwall, KTH Royal Institute of Technology; Shuanglin Chen, CompuTherm LLC

8:30 AM Invited **Some Properties if the Multicomponent Diffusivity Matrix**: John Agren¹; ¹Royal Institute of Technology

9:10 AM Invited A Tale of Two Approaches: From Phase Equilibria to Materials Properties : *Qing Chen*¹; ¹Thermo-Calc Software AB



WEDNESDAY AM

9:50 AM Invited A Diffusion Mobility Database for γ / γ' Co-Superalloys: Carelyn Campbell¹; Kilwon Moon¹; Maureen Williams¹; Greta Lindwall²; ¹National Institute of Standards and Technology; ²Royal Institute of Technology (KTH)

10:30 AM Invited Modeling of Diffusion and Intermetallic Phase Formation in Al-Mg Bimetallic **Structures**

: *Alan Luo*¹; ¹Ohio State University

11:10 AM Invited

An Integrated Computational Materials Engineering (ICME) Framework for Additive Manufacturing (AM) of Ni-based Superalloys: Qiaofu Zhang¹; Abhinav Saboo¹; Jiadong Gong¹; Greg Olson¹; ¹QuesTek Innovations LLC

LIGHT METALS

Magnesium Technology 2021 — Mechanical Behavior

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Petra Maier, University of Applied Sciences Stralsund; J. Brian Jordon, University of Alabama; Neale Neelameggham, IND LLC

Wednesday AM March 17, 2021

Session Chairs: Brian Jordon, University of Alabama; Kiran Solanki, Arizona State

TMS



8:30 AM Invited Quasi-static and Dynamic Rate Mechanical Behavior and Microstructural Investigation of High-purity Mg and AZ31B Alloy: *Benjamin Morrow*¹; Ellen Cerreta¹; Saryu Fensin¹; Sara Perez-Bergquist¹; Carl Trujillo¹; Suveen Mathaudhu²; Veronica Anghel¹; Rodney McCabe¹; George Gray¹; ¹Los Alamos National Laboratory; ²University of California - Riverside

9:00 AM Invited Understanding Twinning: Detwinning Behavior of Unalloyed Mg during Lowcycle Fatigue Using High Energy X-ray Diffraction: Aeriel Murphy-Leonard¹; John Allison²; ¹Naval Research Laboratory; ²University of Michigan

9:30 AM

The Effects of Basal and Prismatic Precipitates on Deformation Twinning in AZ91 **Magnesium Alloy**: Brandon Leu¹; M Arul Kumar²; Irene Beyerlein¹; ¹University of California Santa Barbara; ²Los Alamos National Laboratory

9:50 AM

On the Role of Crystallographic Anisotropy and Texture in Damage Tolerance of Magnesium and its Alloys: Shahmeer Baweja¹; Padmeya Indurkar²; Shailendra Joshi¹; ¹University of Houston; ²National University of Singapore

10:10 AM Invited Achieving Excellent Room Temperature Formability and High Strength in Wrought Magnesium Alloy Sheets: Taisuke Sasaki¹; Zehao Li¹; Kazuhiro Hono¹; ¹NIMS

10:40 AM Invited Texture and Microstructure Evolution in Thermomechanically Processed Mg-Ca



and Mg-Zn-Ca Alloys: Tracy Berman¹; John Allison¹; ¹University of Michigan

11:10 AM Eliminating Yield Anisotropy and Enhancing Ductility in Mg Alloys by Shear Assisted Processing and Extrusion: Dalong Zhang¹; Jens Darsell¹; Nicole Overman¹; Darrell Herling¹; Vineet Joshi¹; ¹Pacific Northwest National Laboratory

11:30 AM Numerical Study of Multi-axial Loading Behavior of Mg Alloy AZ31 Extruded Bar: Huamiao Wang¹; Xiaodan Zhang¹; ¹Shanghai Jiao Tong University

NUCLEAR MATERIALS

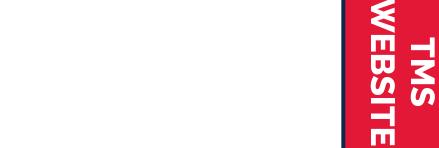
Materials and Chemistry for Molten Salt Systems — Salt Structure and **Properties**

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short, Massachusetts Institute of Technology; Raluca Scarlat, University of California-Berkeley

Wednesday AM March 17, 2021

Session Chair: Raluca Scarlat, UC Berkeley



8:30 AM

Development of Higher Order Systems for the Molten Salt Thermodynamic **Database and their Application**: *Theodore Besmann*¹; Kaitlin Johnson¹; Johnathan Ard¹; Jacob Yingling¹; Matthew Christian¹; Juliano Schorne-Pinto¹; Mahmut Aslani¹; Jake McMurray²; Max Poschmann³; Markus Piro³; ¹University of South Carolina; ²Oak Ridge National Laboratory; ³Ontario Tech

8:50 AM

Ab Initio Molecular Dynamics Simulations of Actinide Molten Chloride Salts: David Andersson¹; ¹Los Alamos National Laboratory

9:10 AM

Extracting Salt Properties from Visualization of Molten Salt Sessile Droplets: Sara Mastromarino¹; Malachi Nelson¹; Raluca Scarlat¹; *Ryan Hayes*²; ¹University of California Berkeley; ²University of California, Berkeley

9:30 AM

Liquid-vapor Equilibrium and Transport Phenomena in Molten Salt Systems: Jacob Mcmurray¹; Joanna McFarlane¹; Scott Greenwood¹; Abbey McAlister¹; Matt Kurley¹; ¹Oak Ridge National Laboratory

9:50 AM

Optimization of the Phase Equilibria and Thermodynamics for Rare-earth Fluoride Systems Relevant to Molten Salt Reactors: Kaitlin Johnson¹; Juliano Schorne Pinto¹; Theodore Besmann¹; ¹University Of South Carolina

10:10 AM

Molten Salt Reactor: Fluoride/Chloride Salt Comparison: Sylvie Delpech¹; Céline Cannes¹; Davide Rodrigues¹; ¹IJCLAB-CNRS



10:40 AM

X-ray Absorption Studies Investigating Solute-solvent Interactions in Molten Salt **Environments**: Elaine Dias¹; *Simerjeet Gill*¹; Ruchi Gakhar²; Santanu Roy³; Mehmet Topsakal¹; William Phillips²; Bobby Layne¹; Shannon Mahurin³; Phillip Halstenberg³; James Wishart¹; Vyacheslav Bryantsev³; Anatoly Frenkel¹; ¹Brookhaven National Laboratory; ²Idaho National Laboratory; ³Oak Ridge National Laboratory

11:00 AM

Imaging Nanostructural Heterogeneities Induced by Molten Salt Corrosion in **Ni-Cr Alloy**: *Yang Yang*¹; Weiyue Zhou²; Sheng Yin¹; Sarah Wang³; Qin Yu¹; Robert Ritchie¹; Mark Asta¹; Ju Li²; Michael Short²; Andrew Minor¹; ¹Lawrence Berkeley National Laboratory; ²Massachusetts Institute of Technology; ³University of California, Berkeley

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Material Processing and Recycling

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao, University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology Company Ltd.; Shadia Ikhmayies

Wednesday AM March 17, 2021

- TMS WEBSITE

8:30 AM Investigation of Nickel Laterite Smelting Slags: Ender Keskinkilic¹; ¹Atilim University

8:50 AM

Recycled Common Glass Bottle Used in Composite Repair for Industrial Piping: *Felipe Lopes*¹; Noan Tonini Simonassi¹; Carlos Fontes Vieira¹; Sergio Neves Monteiro¹; ¹Universidade Estadual do Norte Fluminense

9:10 AM

The Effect of the Diameter on the Density of Ubim Fiber: *BELAYNE MARCHI*¹; Sergio Monteiro²; Veronica Cândido¹; Raphael Reis¹; ¹Instituto Militar de Engenharia; ²Instituto Militar de Engenharia

9:30 AM Invited Effect of Temperature on the Leachability of Chromium in EAF Slag: Ya-Jun Wang¹; Jun-Guo Li¹; Ya-Nan Zeng¹; Zhi-Yuan Gao²; ¹North China University of Science and Technology; ²Tangshan research academy of environmental planning

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and Beyond — Superalloys: Processing

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee



WEDNESDAY AM

TABLE OF

NTENTS

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Wednesday AM March 17, 2021

8:30 AM Keynote Considerations for Manufacturability and Repairability of Next Generation High Temperature Alloys: *Rob Proctor*¹; ¹Rolls-Royce Corporation

9:10 AM

Observation of Multiply Coherent Grains in Ni-Based Superalloy LSHR: *Cameron Hale*¹; Brady Dowdell²; Victoria Miller¹; ¹University of Florida; ²North Carolina State University

9:30 AM

Feasibility of Near-net-shape HIP Fabrication and PM/Wrought Weld in Alloy IN74OH for AUSC Components: *Shenyan Huang*¹; Victor Samarov²; Jack deBarbadillo³;TimothyHanlon¹;BethLewis⁴;RonnieGollihue³;JohnShingledecker⁵; Jason Mortzheim¹; ¹GE Research; ²Synertech PM Inc.; ³Special Metals; ⁴Wyman-Gordon; ⁵Electric Power Research Institute

9:50 AM Invited

Understanding the Effects of Alloy Chemistry and Microstructure on the Stress Relaxation Behavior of High Strength Ni-base Superalloys: Sammy Tin¹; ¹Illinois



TMS WEBSITE

10:20 AM

Synchrotron X-Ray Scattering Characterization of Strengthening Precipitates in a Model Ni-based Alloy: Matthew Frith¹; John Chiles²; Jonathan Poplawsky²; Jan Ilavsky¹; Govindarajan Muralidharan²; ¹Argonne National Laboratory; ²Oak Ridge National Laboratory

10:40 AM

On the Early Stages of Gamma' Evolution in a Model Ni-based Alloy: Govindarajan *Muralidharan*¹; Shivakant Shukla¹; John Chiles¹; Dean Pierce¹; Larry Allard¹; Balasubramaniam Radhakrishnan¹; Jonathan Poplawsky¹; ¹Oak Ridge National Laboratory

MATERIALS PROCESSING

Materials Processing Fundamentals — Thermodynamics on Metals and Slags **Processing**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Process Technology and Modeling Committee

Program Organizers: Jonghyun Lee, Iowa State University; Samuel Wagstaff, Oculatus; Alexandra Anderson, Gopher Resource; Fiseha Tesfaye, Abo Akademi University; Guillaume Lambotte, Boston Metal; Antoine Allanore, Massachusetts Institute of Technology



Session Chairs: Guillaume Lambotte, Boston Metal; Fiseha Tesfaye, Åbo Akademi University

8:30 AM

Effect of Slag Conductivity on Decarburisation Reaction Kinetics: Jayasree *Biswas*¹; Kenneth Coley²; ¹McMaster University; ²Western University

8:50 AM

Experimental Characterization of Liquid Metal Bubble-driven Flows Modeling the Situation in a Steel Ladle

: Thomas Wondrak¹; Christian Bruch²; *Sven Eckert*¹; Pascal Gardin³; Gernot Hackl⁴; Helmut Lachmund⁵; Hans-Bodo Lüngen⁶; Hans-Jürgen Odenthal⁷; Klaus Timmel¹; Bernd Willers¹; ¹Helmholtz-Zentrum Dresden-Rossendorf; ²Saarstahl AG; ³ArcelorMittal; ⁴RHI-Magnesita; ⁵Dillinger Hüttenwerke; ⁶Steel Institute VDEh; ⁷SMS group GmbH

9:10 AM

Influence of Slab Transportation and Handling Practice on Crack Sensitivity of Micro-alloyed Steels: Hossam Shafy¹; Heinz Palkowski¹; ¹Clausthal University of Technology

9:30 AM

Low Temperature Aluminothermic Reduction of Metal Oxides: Jawad Haidar¹; ¹Kinaltek Pty Ltd.

9:50 AM

Modelling of Metal Loss in Ferromanganese Furnace Tapping Operations: Quinn *Reynolds*¹; Jan Erik Olsen²; ¹Mintek; ²SINTEF Industry

10:10 AM

Carbothermal Reduction of Brazilian Linz Donawitz-LD Steel Sludges: Mery Gomez-Marroquin¹; Jose Carlos D'Abreu²; Enrique Dionisio-Calderón²; Nilton

NTENTS

Π

9

Cárdenas-Falcón³; Abraham Terrones - Ramirez⁴; Jhony Huarcaya-Nina⁵; Kim Phatti - Satto⁴; Fernando Huaman-Perez⁶; ¹APMMM/Universidad Nacional de Ingeniería; ²Pontifícia Universidade Católica do Rio de Janeiro ; ³Pontificia Universidad Católica del Perú ; ⁴FIGMM Universidad Nacional de Ingeniería; ⁵FIA Universidad Nacional

de Ingeniería; ⁶FIQT Universidad Nacional de Ingeniería

10:30 AM

Liquid-liquid Extraction Thermodynamic Parameter Estimator (LLEPE) for Multicomponent Separation Systems: *Titus Quah*¹; Chukwunwike Iloeje¹; ¹Argonne National Laboratory

10:50 AM

Thermodynamic Modeling of Iron-copper-sulfuric Acid Solutions during Solvent **Extraction and Electrowinning for Copper Production**: *Jiahao Xu*¹; Guikuan Yue¹; ¹University of Texas El Paso

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Early Career

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb



Massey, Oak Ridge National Laboratory

Wednesday AM March 17, 2021

8:30 AM Invited On the Role of Material Pedigree to Predict Engineering Material Properties: Andrea Rovinelli¹; Mark Messner¹; T.-L. Sham¹; ¹Argonne National Laboratory

8:50 AM Invited A Model for Dislocation Climb and Precipitate Interactions Applied to Creep in Ferritic Steel: Aaron Kohnert¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

9:10 AM Invited Atom-probe Study of Nano-hardening Features in Neutron Irradiated RAFM

Steels: Arunodaya Bhattacharya¹; Philip Edmondson¹; Hiroyasu Tanigawa²; Takashi Nozawa²; Josina Geringer¹; Yutai Katoh¹; Michael Rieth³; ¹Oak Ridge National Laboratory; ²National Institutes for Quantum and Radiological Science and Technology; ³Karlsruhe Institute of Technology

9:30 AM Invited

Microstructural Effects on the Mechanical Behavior of FeCrAl Alloys: Andrew *Hoffman*¹; Shenyan Huang¹; Steve Buresh¹; Michael Schuster¹; Evan Dolley¹; Raul Rebak¹; ¹GE Research

9:50 AM Invited

NovelSmallScaleMechanicalTestingTechniquesforNuclearMaterials: Jonathan *Gigax*¹; Hyosim Kim¹; Calvin Lear¹; Matthew Chancey¹; Peter Hosemann²; Yongqiang Wang¹; Stuart Maloy¹; Nan Li¹; ¹Los Alamos National Lab; ²University of California-Berkeley



MOBILE-FRIEND

Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

CHARACTERIZATION

Connecticut

10:10 AM Invited

10:30 AM Invited

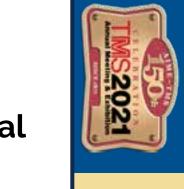
Mechanical Response of Materials Investigated through Novel In-situ

11:10 AM Invited The Merit of In-situ Environmental TEM for the Study of Tungsten under Fusionrelevant Conditions: Maanas Togaru¹; Rajat Sainju¹; Yuanyuan Zhu¹; ¹University of

10:50 AM Invited Atomistic Simulations and Theoretical Modelling of the Yield Behavior of Industrial Tantalum Alloys: *Divya Singh*¹; Satish Rao²; Jaafar El-Awady¹; ¹Johns Hopkins University; ²UES Inc.

Small Scale Mechanical Testing of Nuclear Fuel and Cladding: David Frazer¹; Joshua White²; Tarik Saleh²; Fabiola Cappia¹; Fei Teng¹; Daniel Murray¹; Cameron Howard¹; Colin Judge¹; ¹Idaho National Lab; ²LANL

ProbingtheMechanicalBehaviorofIrradiatedMaterialsthroughMicromechanical Testing: *Sezer Ozerinc*¹; ¹Middle East Technical University



WEDNESDAY AM

TABLE

Q

ONTENTS

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

Wednesday AM March 17, 2021

Experiments and Modeling – Session V

Session Chair: Shailendra Joshi, University of Houston

8:30 AM

Complementary In-situ Methods for Crack Evaluation within High-temperature **Materials at Ambient Conditions**

: *Michael Burtscher*¹; Markus Alfreider¹; Michael Wurmshuber¹; Klemens Schmuck¹; Helmut Clemens²; Svea Mayer¹; Daniel Kiener¹; ¹Montanuniversität Leoben; ² Montanuniversität Leoben

8:50 AM

In-situ Experimental Evaluation of Residual Stresses in Composites during Autoclave Manufacturing: Sandeep Chava¹; Sirish Namilae¹; Marwan Al-Haik¹; ¹Embry-Riddle Aeronautical University

9:10 AM

In-situ Investigation of Intergranular Crack Initiation in Hydrogen Embrittled **Inconel 725**: *Mengying Liu*¹; Lai Jiang¹; Emmeline Sheu¹; Michael Demkowicz¹; ¹Texas A&M University

9:30 AM

Advanced In-situ Electrochemical Nanoindentation Testing for Understanding Hydrogen-materials Interactions: Verena Maier-Kiener¹; Anna Ebner¹; Helmut Clemens¹; Reinhard Pippan²; ¹Montanuniversitaet Leoben; ²Austrian Academy of

Sciences

9:50 AM

Size Effects in Barium Titanate: Nidhin Mathews¹; Ashish Saxena²; Christoph Kirchlechner²; N Venkataramani¹; Gerhard Dehm²; Balila Nagamani Jaya¹; ¹Indian Institute of Technology Bombay; ²Max-Planck-Institut für Eisenforschung GmbH

10:10 AM

Size Effect, Friction and Adhesion in Small-scale Cutting of Metals: Gan Feng¹; Parth Dave¹; Dinakar Sagapuram¹; ¹Texas A&M University

10:30 AM

The Effect of Material Volume on Impact Energy Absorption for Protective Equipment Applications: Kendra Hartley¹; Prasad Tennakoon²; John Nychka¹; ¹University of Alberta; ²Superior Glove Works, Ltd.

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — **Pyrometallurgy** I

Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers;

Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

Wednesday AM March 17, 2021

8:30 AM

One-step Extraction of Nickel from Nickel Sulfide Concentrates by Iron Addition: *Fanmao Wang*¹; Sam Marcuson¹; Leili Khajavi²; Mansoor Barati¹; ¹University of Toronto; ²University of British Columbia

8:50 AM

Continuous Improvement of Process Advisor Optimizing Furnace Model: Peter *Björklund*¹; David Grimsey²; Mikko Korpi¹; Miikka Marjakoski³; ¹Outotec; ²BHP; ³Boliden

9:10 AM

Fluxing Optimisation and Control Improvements at the Kalgoorlie Nickel Smelter: David Grimsey; Eric Grimsey¹; Peter Björklund²; ¹Curtin University; ²Outotec

9:30 AM

Preparation of Refractory Materials by Co-sintering of Ferronickel Slag and Ferrochromium Slag: Thermodynamic Analysis: Foquan Gu¹; Yuanbo Zhang¹; Zhiwei Peng¹; Huimin Tang¹; Zijian Su¹; Tao Jiang¹; ¹Central South University

9:50 AM

PGM Furnace Design, Construction, Improvement and Performance Optimisation: Isobel McDougall¹; Gerrit de Villiers¹; *Hugo Joubert*¹; Burger van Beek²; John Davis²; Trevor Goff²; ¹Tenova Pyromet; ²Sibanye-Stillwater



ELECTRONIC MATERIALS



Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Alloy Phases Committee**

Program Organizers: Hiroshi Nishikawa, Osaka University; Shih-kang Lin, National Cheng Kung University; Chao-Hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jaeho Lee, Hongik University; Zhi-Quan Liu, Shenzhen Institutes of Advanced Technology; Ming-Tzer Lin, National Chung Hsing University; Dajian Li, Karlsruhe Institute of Technology; Yu Zhong, Worcester Polytechnic Institute; Yee-wen Yen, National Taiwan University of Science and Technology; A.S.Md Abdul Haseeb, University of Malaya; Ligang Zhang, Central South University; Sehoon Yoo, KITECH; Vesa Vuorinen, Aalto University; Yu-chen Liu, National Cheng Kung University

Wednesday AM March 17, 2021

Session Chairs: Shih-kang Lin, National Cheng Kung University; Yee-Wen Yen, National Taiwan University of Science and Technology

8:30 AM Introductory Comments: Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XX: Sinn-wen Chen¹; ¹National Tsinghua University

8:35 AM Keynote Interfacial Reactions in the Bi2Te3 Thermoelectric Modules: Sinn-wen Chen¹; Ya-Hsiang Hsu¹; Hao-wei Shih¹; ¹National Tsing Hua University

9:15 AM Invited

Review of X-ray Microbeam Study of Electromigration: *Ping-Chuan Wang*¹; ¹SUNY New Paltz

9:45 AM

Effects of Bromide and Adipic Acid on Electrochemical Migration of Tin: A.S.Md Abdul Haseeb¹; Ee Lynn Lee¹; Yi Sing Goh¹; Y. H. Wong¹; M. F. M. Sabri¹; B. Y. Low²; ¹University of Malaya; ²NXP Semiconductor Sdn Bhd

10:05 AM

The Microstructure and Properties Variations of Sn-coated Cu Wires Induced by Electromigration: Hsiao-Chun Liu¹; Chien-Lung Liang¹; Tsung-Chieh Chiu²; Kwang-Lung Lin¹; ¹National Cheng Kung University; ²Conquer Electronics

10:25 AM

Thermomigration Failure Induced by Surface Diffusion of Sn on Ni/Cu Metallization in Microbumps for 2.5-dimensional Integrated Circuits Packaging: *Wei-Dung Tsai*¹; Chen Wei Lee¹; Fan-Yi Ouyang¹; ¹National Tsing Hua University

10:45 AM

Synchrotron White Laue Nanodiffraction Characterization of Allotropic Phase Transformation of Hexagonal- into Monoclinic-Cu₆Sn_{5: Pei-Tzu Lee}¹; Wan-Zhen Hsieh²; Cheng-Yu Lee³; Yu-Hsuan Huang³; Ching-Yu Chiang²; Ching-Shun Ku²; C. Robert Kao¹; Cheng-En Ho³; ¹National Taiwan University; ²National Synchrotron Radiation Research Center; ³Yuan Ze University

11:05 AM

TMS

Electroplating of NiP for the Low Residual and High Strength MEMS Probe Tip:

Na-Young Kang¹; *Jaeho Lee*¹; ¹Hongik University



WEDNESDAY AM

O

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Non-Ferrous Alloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Wednesday AM March 17, 2021

Session Chair: Deep Choudhuri, New Mexico Institute of Mining and Technology

8:30 AM

Effect of Zirconium Addition to Wrought Al-Mg-Si Alloys on Microstructure: Florian Schmid¹; Irmgard Weißensteiner²; Matheus Tunes²; Thomas Kremmer²; Thomas Ebner³; Peter J. Uggowitzer²; Stefan Pogatscher²; ¹Christian Doppler Laboratory for Advanced Aluminum Alloys; ²Montanuniversitaet Leoben; ³AMAG rolling GmbH

8:50 AM

MOBILE-FRIEND

Phase Transitions in Beta Ti and Beta Zr Alloys: Josef Strasky¹; Anna Veverková¹; ¹Charles University

9:10 AM

Local Phase Transformation Strengthening in Ni-based Superalloys: Ashton *Egan*¹; Timothy Smith²; You Rao¹; Longsheng Feng¹; Emmanuelle Marquis³; Maryam Ghazisaeidi¹; Yunzhi Wang¹; Steve Niezgoda¹; Michael Mills¹; ¹Ohio State University; ²NASA Glenn Research Center; ³University of Michigan

9:30 AM

On the Application Potential of Aluminum Crossover Alloys: Lukas Stemper¹; Matheus Tunes¹; Ramona Tosone²; Peter Uggowitzer¹; Stefan Pogatscher¹; ¹Montanuniversitaet Leoben; ²AMAG rolling GmbH

9:50 AM

Thermal Behavior and Decomposition of Quasicrystalline Dispersoids in Powderprocessed Aluminum Alloys: Hannah Leonard¹; Sarshad Rommel¹; Mingxuan Li¹; Thomas Watson²; Tod Policandriotes³; Mark Aindow¹; ¹University of Connecticut; ²Pratt & Whitney; ³Collins Aerospace

MATERIALS PROCESSING

Rare Metal Extraction & Processing — Recycling, Co, REE



Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

Wednesday AM March 17, 2021

8:30 AM

Recycling of Rare Earths from Neodymium Magnets Using Focused Infrared and Solid Phase Extraction: *Mélodie Bonin*¹; Dominic Larivière¹; ¹Université Laval

8:50 AM Invited

The Italian National Research Council Operations within the EIT Raw Materials **Framework**: *Paolo Dambruoso*¹; Salvatore Siano²; Armida Torreggiani¹; Ornella Russo³; Vladimiro Dal Santo⁴; Stefania Marzocchi⁵; ¹ISOF-CNR; ²IFAC-CNR; ³Library of the Bologna CNR Research Area ; ⁴SCITEC-CNR; ⁵Library of the Bologna CNR **Research** Area

9:10 AM

Experimental Determination of Liquidus Temperature and Phase Equilibria of the CaO-Al₂O₃-SiO₂-Na₂O Slag System Relevant to E-waste Smelting: Md Khairul *Islam*¹; Michael Somerville²; Mark Pownceby²; James Tardio¹; Nawshad Haque²; Suresh Bhargava¹; ¹RMIT University; ²CSIRO

9:30 AM Invited

ONTENTS

FABLE OF



WEDNESDAY AM

How to Prepare Future Generations for the Challenges in the Raw Materials Sector: Armida Torreggiani¹; Alberto Zanelli²; Alessandra Degli Esposti²; Eleonora Polo²; Paolo Dambruoso²; Renata Lapiska-Viola²; Kerstin Forsberg³; Emilia Benvenuti⁴; ¹National Research Council of Italy-CNR; ²ISOF- CNR; ³KTH - Royal Institute of Technology; ⁴National Research Council of Italy (CNR)

9:50 AM Invited Circular Economy for Rare Earths: What are the Different Strategies, Challenges, and Opportunities?: *Komal Habib*¹; ¹University of Waterloo

ENERGY & ENVIRONMENT

Recycling and Sustainability for Emerging Technologies and Strategic Materials — Recycling and Process Optimization I

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: John Howarter, Purdue University; Mingming Zhang, ArcelorMittal Global R&D; Elsa Olivetti, Massachusetts Institute of Technology; Hong Peng, University of Queensland

Wednesday AM March 17, 2021

Session Chair: Hong Peng, University of Queensland

8:30 AM **Copper Separation from Steel Scrap**: *Hyunsoo Jin*¹; Brajendra Mishra¹; ¹Worcester Polytechnic Institute



Thermal Property Characterization, Modeling, and Theory in Extreme

8:50 AM

Improvement of Steel Scrap Recycling: Optical Recognition of Cu Impurities Using Machine Learning: *Zhijiang Gao*¹; ¹Colorado School of Mines

9:10 AM

Copper Supply for Electric Vehicles and Impacts on the Recycling Sector: Ayomipo Arowosola¹; Gabrielle Gaustad²; ¹Rochester Institute of Technology; ²Alfred University

9:30 AM

Development and Impact of High-performance Al Alloys Alloyed with Rare Earth **Co-products**: *Hunter Henderson*¹; Zachary Sims²; David Weiss³; Tomer Fishman⁴; Ryan Ott⁵; Orlando Rios²; Scott McCall¹; ¹Lawrence Livermore National Laboratory; ²University of Tennessee-Knoxville; ³Eck Industries, Inc.; ⁴IDC Herzliya; ⁵Ames Laboratory

9:50 AM

Electrochemical Separation of Aluminum from Mixed Scrap Using Ionic Liquids: Aninda Nafis Ahmed¹; Ramana Reddy¹; ¹The University of Alabama

10:10 AM

High-temperature Oxidation of Explosion Welded Tantalum-tungsten Alloy on Steel Substrate as a Potential Technique for Recycling: Akanksha Gupta¹; Brajendra Mishra¹; ¹Worcester Polytechnic Institute

NUCLEAR MATERIALS

Environments — Early Career Scholars in Thermal Properties

Sponsored by: TMS Structural Materials Division, TMS: Nuclear Materials Committee

Program Organizers: Janelle Wharry, Purdue University; Mukesh Bachhav, Idaho National Laboratory; Marat Khafizov, Ohio State University; Eric Lass, University of Tennessee-Knoxville; Vikas Tomar, Purdue University; Tiankai Yao, Idaho National Laboratory; Cody Dennett, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Wednesday AM March 17, 2021

Session Chairs: Cody Dennett, Idaho National Laboratory; Fergany Badry, Texas A&M University

8:30 AM Invited A Thermodynamically-consistent Model for Heat Transport in Heterogeneous **Solids**: *Karim Ahmed*¹; Fergany Badry¹; ¹Texas A&M University

8:55 AM Invited

Defect Density and Annealing Kinetics Estimation Using Thermal Diffusivity Measurements from Transient Grating Spectroscopy: Mohamed Abdallah *Reza*¹; Hongbing Yu¹; Kenichiro Mizohata²; Felix Hofmann¹; ¹University Of Oxford; ²University of Helsinki

9:20 AM Invited

Thermal Behaviors of Correlated Insulators ThO2 and SmB6: Narayan Poudel¹; Daniel Murray¹; Matthew Mann²; Jason Jeffries³; Krzysztof Gofryk¹; ¹Idaho National Laboratory; ²Air Force Research Laboratory; ³Lawrence Livermore National

TMS



TMS-DGM Symposium: A Joint US-European Symposium on Linking Basic Science to Advances in Manufacturing of Lightweight Metals — Session I

9:45 AM Invited

Thermal Conductivity Degradation from Irradiation-induced Microstructural **Defects in Single Crystal Thorium Dioxide**: Amey Khanolkar¹; Zilong Hua¹; Cody Dennett¹; Marat Khafizov²; Tiankai Yao¹; Kaustubh Bawane¹; Lingfeng He¹; J. Matthew Mann³; Anter El-Azab⁴; Jian Gan¹; David Hurley¹; ¹Idaho National Laboratory; ²Ohio State University; ³Air Force Research Laboratory; ⁴Purdue University

10:10 AM Invited

Phase-dictated Thermal Conductivity Response in Carbon Systems Exposed to Ion Irradiation: *Ethan Scott*¹; Khalid Hattar²; Jeffrey Braun¹; Sean King³; Mark Goorsky⁴; Patrick Hopkins¹; ¹University of Virginia; ²Sandia National Laboratories; ³Intel Corporation ; ⁴University of California Los Angeles

10:35 AM Invited

Thermal Transport Behavior of U-50Zr at the Mesoscale: Before and After Irradiation: *Zilong Hua*¹; Tiankai Yao¹; Amey Khanolkar¹; Cody Dennett¹; Xiaxin Ding¹; Krzysztof Gofryk¹; Michael Benson¹; Lingfeng He¹; Jian Gan¹; David Hurley¹; ¹Idaho National Laboratory

11:00 AM Invited **Non-magnetic Kondo Effect in Eelta-UZr2**: *Xiaxin Ding*¹; Kaya Wei²; Tiankai Yao¹; Ryan Baumbach²; Krzysztof Gofryk¹; ¹Idaho National Laboratory; ²National High Magnetic Field Laboratory

LIGHT METALS

CONTENTS

TABLE

Q



Sponsored by: Deutsche Gesellschaft für Materialkunde e.V. (DGM): German Materials Society, TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee

Program Organizers: William Joost; Norbert Hort, Helmholtz-Zentrum Geesthacht

Wednesday AM March 17, 2021

Session Chair: William Joost, Pratt & Whitney

8:30 AM

Stacking-fault Mediated Plasticity and Strengthening in Lean, Rare-earth Free Magnesium Alloys: Indranil Basu¹; Jörg Löffler¹; ¹ETH Zurich

8:50 AM

High-throughput Evaluation of Hardening Potency and Solubility of Eight Alloying Elements in Magnesium: Chuangye Wang¹; Wei Zhong¹; Ji-Cheng Zhao¹; ¹University Of Maryland

9:10 AM

High-throughput Experimental Techniques to Measure the CRSS for Slip and Twinning in Mg and Mg Alloys: Jingya Wang¹; Reza Alizadeh²; Javier Llorca³; ¹Shanghai Jiao Tong University and IMDEA Materials Institute; ²Sharif University of Technology and IMDEA Materials Institute; ³IMDEA Materials Institute & Technical University of Madrid

9:30 AM

Study of the Solidification Pathways of Hypo/hyper-eutectic Al-Ce over a Wide

TMS

Range of Thermal Histories: Akankshya Sahoo¹; Abdoul Aziz Bogno¹; Hani Henein¹;

¹University of Alberta

WEDNESDAY PM

TABLE ONTENTS Q

9:50 AM

Solute-vacancy Clustering in Aluminum: Dongwon Shin¹; Jian Peng¹; Sumit Bahl¹; Amit Shyam¹; James Haynes¹; ¹Oak Ridge National Laboratory

10:10 AM

Fracture Mechanisms under Monotonic Tensile, Fatigue, and Creep Deformation of Cast Al-Cu-Mn-Zr Alloys: Impact of Brittle Intermetallic Grain Boundary **Particles**: *Sumit Bahl*¹; Xiaohua Hu¹; Jiahao Cheng¹; Eric Hoar²; Kevin Sisco³; Richard Michi¹; J. Allen Haynes¹; Amit Shyam¹; ¹Oak Ridge National Laboratory; ²Georgia Institute of Technology; ³University of Tennessee-Knoxville

10:30 AM

Al-Fe-Si Phase Stabilization Using Experimentally Validated Computational **Thermodynamics**: *Sujeily Soto-Medina*¹; Biswas Rijal¹; Lilong Zhu²; Richard Hennig¹; Michele Manuel¹; ¹University of Florida; ²Yantai University

10:50 AM

Spatial Correlations between Strengthening Particles in Multi-phase Hardenable Aluminum Alloys: Viktor Wessely¹; Robin Schäubin¹; Stephan Gerstl¹; Stefan Pogatscher²; Peter Uggowitzer¹; Jörg Löffler¹; ¹Laboratory of Metal Physics and Technology; ²Montanuniversitaet Leoben,

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Fracture and Modeling

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

Wednesday PM March 17, 2021

Session Chair: Megan Cordill, Erich Schmid Institute

2:00 PM

Characterization of a Novel Crack Growth Mechanism in Ti-6Al-4V Subjected to Dwell Fatigue at Elevated Temperature: Adam Pilchak; John Rotella¹; Nate Levkulich²; Sushant Jha³; Reji John⁴; Jim Larsen⁴; ¹Purdue University and Air Force Research Lab; ²UES Inc.; ³University of Dayton Research Institute; ⁴Air Force **Research Lab**

2:20 PM

The Maximum Limit of Compressive Strength and Hardness of Nanocrystalline MgAl₂O₄ Spinel: Jessica Maita¹; Jacob Davis²; James Wollmershauser³; Edward Gorzkowski³; Boris Feigelson³; Seok-Woo Lee¹; ¹University of Connecticut; ²University of Massachusetts Amherst; ³U.S. Naval Research Laboratory

2:40 PM

Reversing Griffith after 100 Years: Mechanics of the Solid-state Bonding: Yanfei Gao¹; Zhili Feng²; ¹University of Tennessee - Knoxville; ²Oak Ridge National Laboratory



12:45 PM Question and Answer Period

3:00 PM

High-strength and Thermal Stability of Nanotwinned Al Alloys: Qiang Li¹; Sichuang Xue¹; Yifan Zhang¹; Haiyan Wang¹; Jian Wang²; *Xinghang Zhang*¹; ¹Purdue University; ²University of Nebraska-Lincoln

3:20 PM

Nanomechanics of Amorphous Silica: From Mechanical to Fracture Properties: Pania Newell¹; Truong Vo¹; Bang He¹; Michael Blum¹; Angelo Damone²; ¹The University of Utah; ²University of Brescia

SPECIAL TOPICS

2021 TMS Special Sessions — All-conference Plenary

Wednesday PM March 17, 2021

Session Chair: Thomas Battle

12:00 PM

Introductory Comments: Thomas Battle¹; ¹2020 TMS President

12:05 PM

New Methodologies: Producing High-Quality Metal from Low-Grade Ores: Anne Lauvergeon¹; ¹Founder/CEO of ALP; Chair, École des Mines de Nancy; former CEO of Areva S.A.

L



WEDNESDAY PM

MOBILE-FRIEND

SPECIAL TOPICS

2021 TMS Special Sessions – Young Professional Workshop on Preparing a Winning Application Package

Wednesday PM March 17, 2021

2:00 PM Young Professional Workshop on Preparing a Winning Application Package

ADVANCED MATERIALS

2D Materials – Preparation, Properties & Applications – Synthesis, Properties & Applications

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Sufian Abedrabbo, Khalifa University; Amber Shrivastava, Indian Institute of Technology Bombay

Wednesday PM March 17, 2021

Session Chairs: Sufian Abedrabbo, Khalifa University; Nuggehalli Ravindra (Ravi), New Jersey Institute of Technology



Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

NUCLEAR MATERIALS

2:50 PM Invited

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — Multiscale, Physics Based Modeling of Nuclear Materials

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

ONTENTS

TABLE

P

2:00 PM Invited Magnetic and Transport Properties of 2D Layered Chiral Magnets: Junjie Yang¹; ¹New Jersey Institute of Technology

2:25 PM Invited **Elaboration and Characterization of Thin Films of SiP Lamellar Alloys: A First**

Step towards 2D-SiP: Mathieu Stoffel¹; Alix Valdenaire¹; Sébastien Geiskopf¹; Xavier Devaux¹; Erwan André¹; Cedric Carteret¹; Alexandre Bouché¹; Michel Vergnat¹; Hervé Rinnert¹; ¹Universite De Lorraine

Kazue Lopez¹; Arvind Agarwal¹; ¹Florida International University

Polymer Composites Reinforced with 3D Foam of 2D Materials: Tony Thomas¹;



Wednesday PM March 17, 2021

Session Chairs: Benjamin Beeler, North Carolina State University ; Shijun Zhao, City University of Hong Kong

2:00 PM Invited **Overview of Advanced Fuels and Materials R&D within the US DOE-NE NEAMS Program**: Chris Stanek¹; ¹Los Alamos National Laboratory

2:30 PM

Constructing Multi-component Diffusion under Irradiation in U-Mo Alloys: *Benjamin Beeler*¹; Bei Ye²; Yipeng Gao³; Shenyang Hu⁴; ¹North Carolina State University; ²Argonne National Laboratory; ³Idaho National Laboratory; ⁴Pacific Northwest National Laboratory

2:50 PM

Effective Bias for Interstitial Clusters to Cavities in BCC Fe: Yuhao Wang¹; Fei Gao¹; Brian Wirth²; ¹University of Michigan - Ann Arbor; ²University of Tennessee, Knoxville

3:10 PM

Microscale Measurement of Elastic Constants in Ceramics Using Picosecond Ultrasonics for High Throughput Characterization and Atomic Model Validations: Yuzhou Wang¹; David Hurley²; Zilong Hua²; Amey Khanolkar²; Cody Dennett²; Marat Khafizov¹; ¹Ohio State University; ²Idaho National Laboratory

3:30 PM

Effect of Distributed Gas Bubbles on Elastic-plastic Deformation Behavior in **Polycrystalline UMo**: *Shenyang Hu*¹; Benjamin Beeler²; Douglas Burkes¹; ¹Pacific

Northwest National Laboratory; ²North Carolina State University

2:00 PM Invited Automotive-specific Requirements for Additive Manufacturing of Metal Materials: *Tyson Brown*¹; Whitney Poling¹; ¹General Motors

3:50 PM Molecular Dynamics Study of Cascade Overlap Effects in FCC Ni: Samuel Morris¹; Brian Wirth¹; ¹University of Tennessee-Knoxville

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Microstructure-based Fatigue Studies on Additive-Manufactured Materials (Jointly Organized with **Fatigue in Materials Symposium)**

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

Wednesday PM March 17, 2021

Session Chair: Garrett Pataky, Clemson University

TABLE **ONTENTS** Q





WEDNESDAY PM

2:30 PM

Fatigue Crack Growth and Fracture Toughness Behavior of Laser Powder Bed **Fusion Titanium Alloys**: *Jamie Kruzic*¹; Tarik Hasib¹; Xiaopeng Li¹; ¹University of New South Wales

2:50 PM

Fatigue Crack Growth Rate of Electron Beam Melted (EBM) Titanium Alloy (Ti-6Al-4V): Effect of Crystallographic Texture and Internal Porosity: Nik Hrabe¹; Jake Benzing¹; Nick Derimow¹; Tim Quinn¹; Jolene Splett¹; Lucas Koepke¹; ¹National Institute of Standards and Technology

3:10 PM

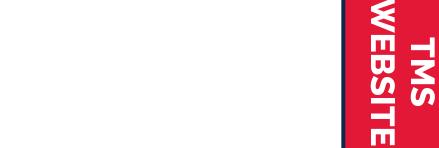
Laser Powder Bed Fusion of Hydride-dehydride Ti-6Al-4V Powders: Effect of Hot Isostatic Pressing on Microstructure and Mechanical Properties: Mohammadreza Asherloo¹; Ziheng Wu²; Srujana Rao Yarasi²; Muktesh Paliwal³; Mike Marucci³; Joe Capone⁴; Anthony Rollett²; Amir Mostafaei¹; ¹Illinois Institute of Technology; ²Carnegie Mellon University; ³Kymera International - Reading Alloys; ⁴Ametek Inc.

3:30 PM

Towards Validation for Computed Tomography Processes for Additive Manufacturing: Griffin Jones¹; Jayme Keist¹; Rachel Reed²; Veeraraghavan Sundar²; ¹The Pennsylvania State University; ²UES Inc.

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Functional, Energy, and Magnetic Materials -**Advanced Manufacturing of Magnetic Materials**



Sponsored by: TMS Functional Materials Division, TMS: Additive Manufacturing Committee, TMS: Magnetic Materials Committee

Program Organizers: Markus Chmielus, University of Pittsburgh; Sneha Prabha Narra, Worcester Polytechnic Institute; Mohammad Elahinia, University of Toledo; Reginald Hamilton, Pennsylvania State University; Iver Anderson, Iowa State University Ames Laboratory

Wednesday PM March 17, 2021

2:00 PM Invited **Development of High-temperature Permanent Magnet Alloys for Additive** Manufacturing: Ryan Ott¹; Emrah Simsek¹; Rakesh Chaudhary¹; Scott McCall²; Alex Baker²; ¹Ames Laboratory/Cmi; ²Lawrence Livermore National Laboratory

2:20 PM

Advanced Design for Lightweighting Wind Power Generators Using Additively Manufactured Hard and Soft Magnets: Latha Sethuraman¹; Ganesh Vijayakumar¹; Shreyas Ananthan¹; Jonathan Keller¹; M.Parans Paranthaman²; ¹National Renewable Energy Laboratory; ²Oak Ridge National Laboratory

2:40 PM

An Additive Manufacturing Design Approach to Achieving High Strength and Ductility in Traditionally Brittle Alloys via Laser Powder Bed Fusion: Andrew *Kustas*¹; Tomas Babuska¹; Kyle Johnson¹; Trevor Verdonik²; Samuel Subia¹; Brandon Krick³; Donald Susan¹; ¹Sandia National Laboratories; ²Lehigh University; ³Florida State University

3:00 PM

Cold Spray of Permanent Magnets: Alexander Baker¹; Richard Thuss²; Nathan Woollett¹; Elis Stavrou¹; Scott McCall¹; Harry Radousky¹; ¹Lawrence Livermore National Laboratory; ²TTEC LLC

3:20 PM

Establishing Fundamentals for Laser Metal Deposition of Functional Ni-Mn-Ga Alloys: Effect of Rapid Solidification on Microstructure and Phase Transformation **Characteristics**: *Emily Flitcraft*¹; Jakub Toman²; Markus Chmielus²; Carolin Fink¹; ¹Ohio State University; ²University of Pittsburgh

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Beyond the Beam II — Material Deposition for Sinter **Densification**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Paul Prichard, Kennametal Inc.; James Paramore, US Army Research Laboratory; Peeyush Nandwana, Oak Ridge National Laboratory; Nihan Tuncer, Desktop Metal

Wednesday PM March 17, 2021

Session Chair: Nihan Tuncer, Desktop Metal

2:00 PM

Wall Thickness Effects on Dimensional Variation, Microstructure, and Mechanical



ONTENTS

TABLE

ę

Arretche¹; Eric Poczatek¹; Yun Bai¹; Hiroko Ohtani¹; Sushmit Chowdhury¹; ¹Ford Motor Company

2:20 PM

Bi-metal Composite Material for Plastic Injection Molding Tooling Applications via Fused Filament Fabrication Process

: *Maxim Seleznev*¹; Joe Roy-Mayhew¹; ¹Markforged Inc.

2:40 PM

Direct Ink Writing of Ceramic Architected Materials: *Raphael Thiraux*¹; Lorenzo Valdevit¹; ¹University of California, Irvine

3:00 PM

Beyond the Beam Additive Manufacturing of Titanium Alloys: James Paramore¹; Brady Butler¹; Matthew Dunstan¹; Daniel Lewis¹; Michael Hurst¹; Laura Moody¹; ¹U.S. **Army Research Laboratory**

3:20 PM

Spatial Architecture of Copper Fillers in Additively Manufactured PLA-matrix **Composite**: *Nazmul Haque*¹; Hadi Noori¹; ¹Oklahoma State University

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Titanium Alloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee,



WEDNESDAY PM

TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

Wednesday PM March 17, 2021

Session Chairs: Raj Banerjee, University of North Texas; Bij-Na Kim, Carpenter Additive

2:00 PM Invited Prediction of Large Regions of Microstructure and Phase Distributions for Additive Manufactured Alloys Prediction of the Microstructure, Resultant Phases and Hardness of Additively Manufactured Ti6Al4V: Shunyu Liu¹; Kyung-min Hong¹; *Yung Shin*¹; ¹Purdue University

2:30 PM

Designing Duplex Microstructures in Additive Manufactured Ti Alloys: An Avenue to Achieve High Strength and Ductility: *Jenniffer Bustillos*¹; Atieh Moridi¹; ¹Cornell University

2:50 PM

Controlled Thermal Post-processing of Additively Manufactured Ti-6Al-4V Parts in Order to Enhance their Mechanical Performance: Frederico Rossi Kaschel¹: Rajani Vijayaraghavan¹; Patrick McNally¹; Mert Celikin¹; Denis Dowling¹; ¹I-Form Advanced Manufacturing Centre



MOBILE-FRIEND

TABLE

P

NTENTS

3:10 PM

Recyclability of Ti-6Al-4V Powders Used in Additive Manufacturing: Perspectives and Outlooks: Nicholas Derimow¹; Nikolas Hrabe¹; ¹National Institute of Standards and Technology

3:30 PM

Microstructure Control in a Beta Titanium Alloy via Selective Laser Melting: Sravya Tekumalla¹; Alex Tan Sui Wei²; Krishnan Manickavasagam²; Matteo Seita¹; ¹Nanyang Technological University; ²Advanced Remanufacturing Technology Centre

3:50 PM

Second Phase Precipitation during AM Processing of Metastable Beta Ti Alloys : *Mohan Sai Kiran Nartu*¹; Srinivas Aditya Mantri¹; Abhishek Sharma¹; Eugene Ivanov²; Kyu Cho³; Brandon McWilliams³; Narendra Dahotre¹; Rajarshi Banerjee¹; ¹University of North Texas; ²Tosoh SMD; ³CCDC, US Army Research Laboratory

4:10 PM

Main Microstructural Characteristics of Ti-6Al-4V Components Produced via Electron Beam Additive Manufacturing (EBAM): Silvia Lopez-Castaño¹; Philippe Emile²; Claude Archambeau²; Florence Pettinari-Sturmel³; Joël Douin³; ¹CEMES-CNRS / Airbus Operations S.A.S.; ²Airbus Operations S.A.S.; ³CEMES-CNRS

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling Deformation — Session VI



WEDNESDAY PM

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Wednesday PM March 17, 2021

2:00 PM Invited

Dominant Microstructural Features for Structural Properties in Additively Manufactured AlSi10Mg: Jay Carroll¹; Christopher Laursen¹; Philip Noell¹; John Emery¹; David Moore¹; Garrett Pataky²; ¹Sandia National Laboratories; ²Clemson University

2:30 PM Invited

Investigation of Porosity, Texture, and Damage Evolution of Additively Manufactured 316L Stainless Steel during In-situ Tensile Loading Using High **Energy X-rays**: Aeriel Murphy-Leonard¹; David Rowenhorst¹; ¹Naval Research Laboratory

3:00 PM

Temperature-dependent Intermittent Microplasticity: Quentin Rizzardi¹; Cameron McElfresh²; Jaime Marian²; Douglas Stauffer³; *Robert Maass*⁴; ¹University of Illinois Urbana Champaign; ²University of California Los Angeles; ³Bruker Nano Surfaces;

TMS

⁴Federal Institute for Materials Research and Testing (BAM)

3:20 PM

Characterization and Modeling of Fatigue-induced Grain Growth in Ultrafine Grained Ni: Alejandro Barrios¹; Ebiakpo Kakandar²; Xavier Maeder³; Gustavo Castelluccio²;OlivierPierron¹;¹GeorgiaInstituteofTechnology;²CranfieldUniversity; ³Empa, Swiss Federal Laboratories for Materials Science and Technology

3:40 PM Invited

Microstructure Evolution of a Stainless Steel Produced via Laser Powder Bed Fusion Subjected to Post-Fabrication Treatments: Gwenaelle Proust¹; Wen Hao Kan²; Quentin Portella³; Mahdi Chemkhi⁴; Magnus Garbrecht¹; Delphine Retraint³; ¹University of Sydney; ²Monash University; ³University of Technology of Troyes; ⁴EPF

4:10 PM

Informing Mechanical Model **Development Using Lower-dimensional Descriptions of Microstructural Evolution**: *Darren Pagan*¹; Gideon Schmidt²; Andy Borum²; Timothy Long²; Matthew Miller²; Armand Beaudoin³; ¹Pennsylvania State University; ²Cornell University; ³Cornell High Energy Synchrotron Source

4:30 PM

Effects of Room Temperature Interface Sliding in TIMETAL-407 (Ti-407): Zachary *Kloenne*¹; Gopal Viswanathan¹; Stoichko Antonov²; Stephen Fox³; Michael Loretto⁴; Hamish Fraser¹; ¹Ohio State University; ²Max-Planck-Institut für Eisenforschung GmbH; ³TIMET; ⁴University of Birmingham

4:50 PM

Combined In-situ Neutron and Synchrotron X-ray Diffraction Study of Tensile **Deformation and Texture Evolution in a Magnesium Alloy**: *Tingkun Liu*¹; Aashish Rohatgi¹; Ke An²; Yang Ren³; Bita Ghaffari⁴; Erin Barker¹; Arun Devaraj¹; ¹Pacific Northwest National Laboratory; ²Oak Ridge National Laboratory; ³Argonne National Laboratory; ⁴Ford Motor Company



WEDNESDAY PM

CONTENTS

TABLE

ę

5:10 PM

Modeling the Effects of Free Surfaces on Twinning Behavior: Brandon Leu¹; M Arul Kumar²; Irene Beyerlein¹; ¹University of California Santa Barbara; ²Los Alamos National Laboratory

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Thin Films and **Nanostructures for Optoelectronics I**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

Wednesday PM March 17, 2021

Session Chairs: Gerald Ferblantier, ICUBE; Ramana Chintalapalle, UTEP

2:00 PM Keynote Multi-photon Microfabrication: from Direct Laser Writing to 4D Microprinting: Arnaud Spangenberg¹; ¹IS2M



MOBILE-FRIENDL

CONTENTS

TABLE OF

2:45 PM

Facile Synthesis of 3D Dendritic Gold Nanostructures Assisted by a Templated Growth Process: Application at the Detection of Traces of Molecules: Karine *Mougin*¹; Pierre Bauer¹; ¹Is2m Cnrs

3:10 PM Keynote

Highly Doped Si Metasurfaces Obtained by Coupling Top Down and Out of Equilibrium Approaches: Jean-Marie Poumirol¹; Clément Majorel¹; Nicolas Chery¹; Meiling Zhang¹; Christian Girard¹; Nicolas Mallet²; Filadelfo Cristiano²; Peter Wiecha²; Guilhem Larrieu²; Sébastien Kerdiles³; Anne-Sophie Royet³; Pablo Acosta³; Vincent Paillard¹; Caroline Bonafos¹; ¹Cemes Cnrs; ²LAAS-CNRS; ³CEA-LETI

3:55 PM

Key Mechanical Test Methods to Characterize Optically Clear Adhesives: Mobin Yahyazadehfar¹; Aref Samadi¹; Leopoldo Carbajal¹; Mark Lamontia¹; ¹DuPont

4:15 PM

Spin Coating of Doped-silica on Czochralski-Silicon for Enhanced Radiative **Properties**: Sufian Abedrabbo¹; EL Mostafa Benchafia¹; Anthony Fiory²; Nuggehalli Ravindra²; ¹Khalifa University; ²New Jersey Institute of Technology

ENERGY & ENVIRONMENT

Advanced Magnetic Materials for Energy and Power Conversion Applications - Magnetocaloric and Energy Harvesting

Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee



WEDNESDAY PM

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

Wednesday PM March 17, 2021

Session Chair: Huseyin Ucar, California Polytechnic University

2:00 PM

Bulk-Nano Spark Plasma Sintered Fe-Si-B-Cu-Nb Based Magnetic Alloys: Taban Larimian; Tushar Borkar¹; Varun Chaudhary²; Raju V Ramanujan²; rajeev Gupta³; Jijo Christudasjustus³; ¹Cleveland State University; ²Nanyang Technological University; ³University of Akron

2:20 PM Invited

Characterization of Binder Jet 3D Printed and Direct Laser Deposited Functional Magnetic Materials: Markus Chmielus¹; Jakub Toman¹; Pierangeli Rodriguez de Vecchis¹; Tyler Paplham¹; Aaron Acierno¹; Katerina Kimes¹; Erica Stevens¹; ¹University of Pittsburgh

2:50 PM

Magnetics and Magnetoelastics of Ce-doped Cobalt Ferrite Processed under the Influence of Magnetic Field: Monaji Reddy¹; *Tanjore Jayaraman*²; Neeraj Patil²; Dibakar Das¹; ¹University of Hyderabad; ²University of Michigan-Dearborn

3:10 PM

Magnetoelasic Domains in Fe-Ga Alloys: Matthew Tianen¹; Yongmei Jin¹; ¹Michigan Technological University



2:00 PM

3:30 PM

Overview of Material Thermal Properties for the Advancement of Machine Learning Based Magnetic Design: *Zackery Miller*¹; ¹North Carolina State University

3:50 PM Invited Spin Crossover Complexes as Multicaloric Materials: *Steven Vallone*¹; Karl Sandeman¹; ¹The City University of New York

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Energy Storage with Emphasis on Batteries I

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Wednesday PM March 17, 2021

Session Chairs: Partha Mukherjee, Purdue University; Pallab Barai, Argonne National Laboratory



MOBILE-FRIENDI

Lithium Solid State Batteries as Next Generation Energy Storage Devices: Pallab Barai¹; Anh Ngo¹; Larry Curtiss¹; Venkat Srinivasan¹; ¹Argonne National Laboratory

2:30 PM

A Simple Method to Fabricate Cu6Sn5 Anodes for Lithium-ion Batteries: Xin Tan¹; Qinfen Gu²; Stuart McDonald¹; Kazuhiro Nogita¹; ¹University of Queensland; ²Australian Synchrotron, ANSTO

2:50 PM

Bio-inspired, Machine Learning-enabled Vascular Structures for Fast-Charging Lithium-ion Batteries: *Po-Chun Hsu*¹; ¹Duke University

3:10 PM

Coating Yeast-derived Carbon Nanotubes on Separators to Suppress Li-S Battery Shuttle Effect: Jiajun He¹; Zan Gao¹; *Xiaodong Li*¹; ¹University of Virginia

3:30 PM

Electrochemically Grown Energy Dense Cathodes for Li and Na Ion Battery: *Arghya Patra*¹; Omar Kazi¹; Jerome Davis¹; Beniamin Zahiri¹; Paul Braun¹; ¹University of Illinois at Urbana-Champaign

3:50 PM

Lithium-sulfur Batteries Featuring High Sulfur Loading and Low Electrolyte: Sheng-Heng Chung¹; *Yun-Chung Ho*¹; ¹National Cheng Kung University

4:10 PM

Mesoscale Origin of Morphological Instability in All-Solid-State Lithium Batteries: Bairav Vishnugopi¹; Partha Mukherjee¹; ¹Purdue University

Advanced Real Time Imaging — Mechanical (Joint session with Mechanical



Response of Materials Investigated through Novel In-situ Experiments and Modeling Symposium)

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

Wednesday PM March 17, 2021

Session Chairs: David Alman, USDOE National Energy Technology Laboratory; Robert Wheeler, Microtesting Solutions LLC

2:00 PM Invited **Real Time Studies of the Mechanics of Spherical Microparticles**: Lewei He¹; Xuchen Wang¹; David Veysset²; *Mostafa Hassani*¹; ¹Cornell University; ²MIT

2:20 PM DeterminationofUraniumOxidationKineticsThroughWhite-LightInterferometry:

Yaakov Idell¹; Wigbert Siekhaus¹; Kerri Blobaum¹; William McLean¹; ¹Lawrence Livermore National Laboratory

2:40 PM

The Accurate Measurement of Elastic Modulus and Hardness of Different Crosslinked SU-8 Polymer: Prakash Sarkar¹; Prita Pant¹; Hemant Nanavati¹; ¹Indian Institute of Technology Bombay

3:00 PM

Lubrication Mechanism of Phosphonium Phosphate Ionic Liquid: a Combined In Situ Atomic Force Microscopy and Ex Situ Surface Spectroscopic Study: Filippo *Mangolini*¹; Zixuan Li¹; Oscar Morales-Collazo¹; Jerzy Sadowski²; Hugo Celio¹; Andrei Dolocan¹; Joan Brennecke¹; ¹University of Texas at Austin; ²Brookhaven National Laboratory

3:20 PM Invited

Mapping Local Strains during In Situ SEM Deformation of Nanoporous Materials: Kevin Schmalbach¹; *Nathan Mara*¹; Antonia Antoniou²; ¹University of Minnesota; ²Georgia Institute of Technology

3:40 PM

Local Shock Viscosity Measurement in Composites Using In-situ Time-Gated **Raman Spectroscopy**: *Abhijeet Dhiman*¹; Ayotomi Olokun¹; Nolan Lewis¹; Vikas Tomar¹; ¹Purdue University

CHARACTERIZATION

Advanced Real Time Imaging — Mechanical (Joint session with the 'Mechanical Response of Materials Investigated through Novel In-situ Experiments and Modeling' Symposium)



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Alloy Phases Committee, TMS: Biomaterials Committee

Program Organizers: Jinichiro Nakano, US Department of Energy National Energy Technology Laboratory; David Alman, National Energy Technology Laboratory; Il Sohn, Yonsei University; Hiroyuki Shibata, Imram, Tohoku University; Antoine Allanore, Massachusetts Institute of Technology; Noritaka Saito, Kyushu University; Anna Nakano, US Department of Energy National Energy Technology Laboratory; Zuotai Zhang, Southern University of Science and Technology; Candan Tamerler, University of Kansas; Bryan Webler, Carnegie Mellon University; Wangzhong Mu, KTH Royal Institute of Technology; David Veysset, Stanford University

Wednesday PM March 17, 2021

Session Chairs: David Alman, USDOE National Energy Technology Laboratory; Robert Wheeler, Microtesting Solutions LLC

2:00 PM Invited **Real Time Studies of the Mechanics of Spherical Microparticles**: Lewei He¹; Xuchen Wang¹; David Veysset²; *Mostafa Hassani*¹; ¹Cornell University; ²MIT

2:20 PM

DeterminationofUraniumOxidationKineticsThroughWhite-LightInterferometry: Yaakov Idell¹; Wigbert Siekhaus¹; Kerri Blobaum¹; William McLean¹; ¹Lawrence Livermore National Laboratory



2:40 PM

The Accurate Measurement of Elastic Modulus and Hardness of Different Crosslinked SU-8 Polymer: Prakash Sarkar¹; Prita Pant¹; Hemant Nanavati¹; ¹Indian Institute of Technology Bombay

3:00 PM

Lubrication Mechanism of Phosphonium Phosphate Ionic Liquid: a Combined In Situ Atomic Force Microscopy and Ex Situ Surface Spectroscopic Study: Filippo *Mangolini*¹; Zixuan Li¹; Oscar Morales-Collazo¹; Jerzy Sadowski²; Hugo Celio¹; Andrei Dolocan¹; Joan Brennecke¹; ¹University of Texas at Austin; ²Brookhaven National Laboratory

3:20 PM Invited

Mapping Local Strains during In Situ SEM Deformation of Nanoporous Materials: Kevin Schmalbach¹; *Nathan Mara*¹; Antonia Antoniou²; ¹University of Minnesota; ²Georgia Institute of Technology

3:40 PM

Local Shock Viscosity Measurement in Composites Using In-situ Time-Gated **Raman Spectroscopy**: *Abhijeet Dhiman*¹; Ayotomi Olokun¹; Nolan Lewis¹; Vikas Tomar¹; ¹Purdue University

MATERIALS PROCESSING

Advances in Surface Engineering III — Session II



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee

Program Organizers: Tushar Borkar, Cleveland State University; Arif Mubarok, PPG; Rajeev Gupta, North Carolina State University; Sandip Harimkar, Oklahoma State University; Bharat Jasthi, South Dakota School of Mines & Tech

March 17, 2021 Wednesday PM

Session Chairs: Praful Bari, Oklahoma State University; Tushar Borkar, Cleveland State University

2:00 PM

Electropolishing of Bronze in Concentrated H3PO4: Geng Ni¹; Choong-un Kim¹; ¹University of Texas at Arlington

2:20 PM

Enhancement of Liquid Metal Wetting by Patterning Particles on Oxide Surfaces: Jiyun Park¹; Jason Nicholas²; Yue Qi¹; ¹Brown University; ²Michigan State University

2:40 PM

Magnetron Sputtered Micro-lattice Structures: Expanding the Materials Working **Space of Lattice Materials**: *Alina Garcia Taormina*¹; Chantal Kurpiers²; Andrea Hodge¹; Ruth Schwaiger³; ¹University of Southern California; ²Karlsruhe Institute of Technology; ³Karlsruhe Institute of Technology, Forschungszentrum Juelich GmbH



3:00 PM

ModifyingCorrosionPerformanceofPlasmaElectrolyticOxidation(PEO)Coatings using Potassium Hydroxide (KOH) and Potassium Fluoride (KF) Additives: Navid *Attarzadeh*¹; Maryam Molaei²; Arash Fattah-alhosseini²; ¹University of Texas at El Paso; ²Bu-Ali Sina University

3:20 PM

Nitriding-assisted Surface Enhancement of Multi-

principal Element Alloys: Yu-Hsuan Lin¹; David Poerschke¹; ¹University of Minnesota

3:40 PM

Phase-field Approach on Modeling Wetting of Rough Surfaces: *Dong-Uk Kim*¹; Michael Tonks¹; ¹University of Florida

4:00 PM

The Role of Particle Passivation Layers in the Critical Adhesion Velocity of Cold Sprayed Powders: *Cameron Crook*¹; Lorenzo Valdevit¹; Daniel Mumm¹; Diran Apelian¹; ¹University of California, Irvine

4:20 PM

Trace Element Distributions in Al-Zn Based Coating Alloys on Steel Substrates: Dongdong Qu¹; Matthew Gear¹; Nega Setargew²; Wayne Renshaw²; Stuart McDonald¹; David StJohn¹; David Paterson³; Kazuhiro Nogita¹; ¹The University of Queensland; ²BlueScope Steel Ltd; ³Australian Synchrotron

MATERIALS DESIGN

Advances in Titanium Technology — Phase Transformation and Deformation in **Titanium Alloys**



Sponsored by: TMS Structural Materials Division, TMS: Titanium Committee

Program Organizers: Don Li, Howmet Engineered Products; Yufeng Zheng, University of Nevada-Reno ; Peeyush Nandwana, Oak Ridge National Laboratory; Matthew Dunstan, US Army Research Laboratory

Wednesday PM March 17, 2021

Session Chair: Yufeng Zheng, University of Nevada Reno

2:00 PM

Hierarchical Twinning Microstructure in Beta Titanium Alloys: Dian Li¹; Wenrui Zhao¹; Zachary Kloenne²; Stoichko Antonov³; Dong Wang⁴; Yipeng Gao²; Yunzhi Wang²; Hamish Fraser²; *Yufeng Zheng*¹; ¹University of Nevada, Reno; ²Ohio State University; ³Max-Planck-Institut für Eisenforschung; ⁴Xi'an Jiaotong University

2:20 PM

How Microtextured Regions Influence the Early Slip Activity in Ti Alloys: Samuel Hemery¹; Azdine Naït-Ali¹; Loic Signor¹; Patrick Villechaise¹; McLean Echlin²; Joseph Wendorf²; Jean-Charles Stinville²; Tresa Pollock²; Mikael Gueguen¹; ¹ISAE-ENSMA; ²UCSB

2:40 PM

Influence of Microtextured Regions on Early Plasticity in Ti64: Joseph Wendorf¹; Jean-Charles Stinville¹; Marie-Agathe Charpagne¹; McLean Echlin¹; Andrew Polonsky¹; Paul Dawson²; Tresa Pollock¹; ¹University of California Santa Barbara; ²Cornell University

MOBILE-FRIENDL

3:00 PM

Localization of Plastic Strain in Microtextured Regions of Ti-6Al-4V: Jonathan *Cappola*¹; Jean-Charles Stinville²; Marie-Agathe Charpagne²; Patrick Callahan³; McLean Echlin²; Tresa Pollock²; Adam Pilchak⁴; Matthew Kasemer¹; ¹University of Alabama; ²University of California, Santa Barbara; ³US Naval Research Laboratory; ⁴Air Force Research Laboratory

3:20 PM

Anomalous c+a Dislocation Activity in TIMETAL-407 (Ti-407): Zachary Kloenne¹; Gopal Viswanathan¹; Bo Pang²; Stephen Fox³; Michael Loretto²; Hamish Fraser¹; ¹Ohio State University; ²University of Birmingham; ³TIMET

3:40 PM

Colony Orientation Dependence in the Deformation and Spheroidization of Two-**Phase Titanium Alloys**: *Benjamin Begley*¹; Cameron Frampton¹; Thomas Spradley¹; Jennifer Perez¹; Adam Pilchak²; Victoria Miller¹; ¹University of Florida; ²Air Force **Research Laboratory**

4:00 PM

Effect of Grain Orientation on Slip Transmission in Titanium: An Analysis of Strain Localization within Slip Bands: *Behnam Ahmadikia*¹; Irene Beyerlein¹; ¹University of California, Santa Barbara

MATERIALS DESIGN

AI/Data informatics: Design of Structural Materials — AI/ML Frameworks; **Grain Growth and Simulation Integration**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Jennifer Carter, Case Western Reserve University; Amit Verma, Carnegie Mellon University; Natasha Vermaak, Lehigh University; Jonathan Zimmerman, Sandia National Laboratories; Darren Pagan, Pennsylvania State University; Chris Haines, Ccdc Army Research Laboratory; Judith Brown, Sandia National Laboratories

Wednesday PM March 17, 2021

2:00 PM Invited Data Science Approaches for Microstructure-property Connections in Structural Materials: *Elizabeth Holm*¹; bo Lei¹; Katelyn Jones¹; Ryan Cohn¹; Nan Gao¹; ¹Carnegie Mellon University

2:30 PM Invited Physics-informed Data-driven Machine Learning Approach for Mesoscale **Materials Science**: *Reeju Pokharel*¹; Anup Pandey¹; Alexander Scheinker¹; ¹Los **Alamos National Laboratory**

3:00 PM Invited Combined Statistical and Energetic Approach to Understand Grain Boundary **Embrittlement for Segregation Engineering**: Doruk Aksoy¹; Remi Dingreville²; *Douglas Spearot*¹; ¹University of Florida; ²Sandia National Laboratories



MOBILE-FRIEND

3:30 PM

Machine Learning Approach to Understanding Abnormal Grain Growth: Ryan Cohn¹; Megna Shah²; Adam Pilchak²; Eric Payton²; Anthony Rollett¹; Elizabeth Holm¹; ¹Carnegie Mellon University; ²Air Force Research Laboratory

3:50 PM

Machine Learning for the Recognition and Synthesis of Polycrystalline Metal **Microstructures**: *Neal Brodnik*¹; Devendra Jangid¹; Amil Khan¹; Michael Goebel¹; McLean Echlin¹; B. S. Manjunath¹; Samantha Daly¹; Tresa Pollock¹; ¹University of California Santa Barbara

4:10 PM Invited Using Machine Learning for Targeted Alloy Design in High Entropy Composition **Spaces**: *Tanner Kirk*¹; Richard Couperthwaite¹; Guillermo Vazquez¹; Daniel Sauceda¹; PejmanHonarmandi¹; PrashantSingh²; RaymundoArroyave¹; ¹TexasA&MUniversity; ²Ames Laboratory

4:30 PM

Unsupervised ML to Bridge Molecular Dynamics and Phase field Simulations: *Sukriti Manna*¹; Henry Chan¹; Subramanian Sankaranarayanan¹; ¹Argonne National Laboratory

MATERIALS DESIGN

AI/Data informatics: Tools for Accelerated Design of High-temperature Alloys - High Temperature Mechanical Properties



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Michael Titus, Purdue University; Pinar Acar, Virginia Tech; Andrew Detor, GE Research; James Saal, Citrine Informatics; Dongwon Shin, Oak **Ridge National Laboratory**

Wednesday PM March 17, 2021

Session Chairs: Andrew Detor, GE Research; Dongwon Shin, Oak Ridge National Laboratory; Sudeepta Mondal, Argonne National Laboratory

2:00 PM

Elastic Properties Machine-learning-based Descriptor for a Refractory High **Entropy Alloy**: *Guillermo Vazquez*¹; Prashant Singh²; Daniel Sauceda¹; Raymundo Arroyave¹; ¹Texas A&M University; ²AMES Laboratory

2:20 PM

Predicting Yield Stress of High Temperature Alloys via Computer Vision and Machine Learning: Nan Gao¹; Zongrui Pei²; Youhai Wen²; Michael Gao²; Elizabeth Holm¹; ¹Carnegie Mellon University; ²National Energy Technology Laboratory

2:40 PM

Revealing Nanoscale Features Controlling Diffusion Within Multi-component Alloys through Machine Learning: S. Mohadeseh Taheri-Mousavi¹; S. Sina Moeini-Ardakani¹; Ryan W. Penny¹; Ju Li¹; A. John Hart¹; ¹MIT



MOBILE-FRIEND

3:00 PM

Uncertainty Quantification for Thermo-mechanical Behavior of Aircraft Engine Materials in Elevated Temperatures: Arulmurugan Senthilnathan¹; Pinar Acar¹; ¹Virginia Tech

3:20 PM Invited

Coupling of Data Mining, Thermodynamics and Multi-objective Genetic Algorithms for the Design of High-temperature Alloys: Franck Tancret¹; Edern Menou²; Gérard Ramstein¹; ¹University of Nantes; ²Safran

3:50 PM

Machine Learning Augmented Predictive & Generative Models for Rupture Life in High Temperature Alloys: Madison Wenzlick¹; Osman Mamun²; Ram Devanathan²; Kelly Rose³; Jeffrey Hawk³; ¹Leidos Research Support Team for the National Energy Technology Laboratory; ²Pacific Northwest National Laboratory; ³National Energy Technology Laboratory

4:10 PM

Determining Solute Site Preference and Correlations to Antiphase Boundary Energy in Ni-based Superalloys: *Enze Chen*¹; Tao Wang²; Mario Epler²; Timofey Frolov³; Mark Asta¹; ¹University of California, Berkeley; ²Carpenter Technology Corporation; ³Lawrence Livermore National Laboratory

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering — Computational Simulations and Algorithms for Study Structure-Processing **Relations**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Wednesday PM March 17, 2021

Session Chair: Ebrahim Asadi, University of Memphis

2:00 PM

Real Time Boundary Condition Acquisition and Integration of Heats of Fusion and Phase Transformation Using an Implicit Finite Element Newton Raphson Based Approach for Thermal Behavior Prediction in Additively Manufactured Parts: Deepankar Pal¹; Madhu Keshavamurty¹; Grama Bhashyam¹; ¹Ansys

2:20 PM

Global Local Modeling of Melt Pool Dynamics and Bead Formation in Laser Bed Powder Fusion Process Using a Comprehensive Multi-Physics Simulation: Faiyaz Ahsan¹; Jafar Razmi¹; Leila Ladani¹; ¹Arizona State University

2:40 PM

Multi-scale Modeling of Hierarchical Microstructure in Ceramic Composites: *Matthew Guziewski*¹; David Montes de Oca Zapiain²; Jennifer Synowczynski-Dunn¹; Remi Dingreville²; Shawn Coleman¹; ¹Army Research Laboratory; ²Sandia National Laboratory



3:00 PM

Analysis of Dendrite Growth and Microstructure Evolution during Solidification of Al 6061 via 2D and 3D Phase Field Models: Neil Bailey¹; *Yung Shin*¹; ¹Purdue University

3:20 PM

A Machine Learning Approach for Predicting Melt Pool Size in Wire-feed DED Process: Amit Verma¹; *Zhening Yang*¹; Ali Gruzel¹; Anthony Rollett¹; ¹Carnegie Mellon University

LIGHT METALS

Aluminum Alloys, Processing and Characterization — Processing Innovation, New Applications and Products

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Dimitry Sediako, University of British Columbia

Wednesday PM March 17, 2021

Session Chair: Xiaochun Li, University of California, Los Angeles

2:00 PM

Shear Assisted Processing and Extrusion of Aluminum Alloy 7075 Tubing at High Speed: Scott Whalen¹; Md. Reza-E-Rabby¹; Tianhao Wang¹; Xiaolong Ma¹; Timethy Decendral¹: Decendral¹: Nicolo Overman¹: Prenden Taysem¹: ¹Decifie

Timothy Roosendaal¹; Darrell Herling¹; Nicole Overman¹; Brandon Taysom¹; ¹Pacific

Northwest National Laboratory

Shear Assisted Processing and Extrusion of Thin-walled AA 6063 Tubing: Brandon *Taysom*¹; Scott Whalen¹; MD Reza-E-Rabby¹; Tim Skszek²; Massimo DiCiano²; ¹Pacific Northwest National Laboratory; ²Magna International WEDNESDAY PM

2:40 PM

2:20 PM

Influence of the Quench Rate and Trace Elements on 6XXX Alloys: Alexander *Wimmer*¹; Annika Haemmerle¹; ¹Neuman Aluminium

3:00 PM

The Combined Method for Producing Long Products from Aluminium and **Aluminium Alloys**: *Alexander Salnikov*¹; Christoph Heinzel¹; ¹RUSAL ETC

3:20 PM

Effect of Extrusion Process on Mechanical, Welding and Corrosion Behaviour of 6XXX Series of Aluminium Alloys: *Mehmet Bugra Guner*¹; Murat Konar¹; Görkem Özçelik¹; Tolga Demirkiran¹; ¹Asas Aluminium

3:40 PM

TIG Welding of Dissimilar High-Strength Aluminum Alloys 6061 and 7075 with Nano-treated Filler Wires: Narayanan Murali¹; Xiaochun Li¹; ¹UCLA Department of Materials Science and Engineering

4:00 PM Question and Answer Period

ONTENTS

0



Aluminum Reduction Technology Across the Decades: An LMD Symposium Honoring Alton T. Tabereaux and Harald A. Øye — Harald Øye Honorary Session: Fundamentals in Anode and Cathode Technology - Joint Session with **Electrode Technology**

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Arne Ratvik, SINTEF; Marc Dupuis, GeniSim Inc.; Kristian Etienne Einarsrud, Norwegian University of Science and Technology

Wednesday PM March 17, 2021

Session Chair: Kristian Etienne Einarsrud, 1Norwegian University of Science and Technology (NTNU)

2:00 PM

Introductory Comments: Aluminum Reduction Technology Across the Decades: An LMD Symposium Honoring Alton T. Tabereaux and Harald A. Øye: Kristian *Etienne Einarsrud*¹; ¹Norwegian University of Science and Technology

2:05 PM

Forty Years of Trondheim International Course on Process Metallurgy of **Aluminium**: *Michel Reverdy*¹; Vinko Potocnik²; ¹Emirates Global Aluminium; ²Vinko Potocnik Consultant Inc

2:45 PM

Establishing a Chemical Model of the Melt in the Cathode: Lorentz Petter Lossius¹; Harald Arnljot Øye²; ¹Hydro Aluminium AS; ²NTNU

3:05 PM

Heating New Anodes Using the Waste Heat of Anode Butts Establishing the Interface Thermal Contact Resistance: *Marc Dupuis*¹; Kristian Etienne Einarsrud²;



3:25 PM

Henrik Gudbrandsen²;

Technology (NTNU)

Forty Years of Cathode Block Evolution at EGA: Michel Reverdy¹; Mustafa Mustafa¹; Mohamed Boraie¹; ¹Emirates Global Aluminium

3:45 PM

Wetting of Carbon Cathodes by Molten Electrolyte and Aluminium: Samuel Senanu¹; Arne Petter Ratvik¹; Zhaohui Wang¹; Tor Grande²; ¹SINTEF; ²NTNU Norwegian University of Science and Technology

4:05 PM Question and Answer Period

BIOMATERIALS

Biological Materials Science – Biological Materials Science II

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Biomaterials Committee**

Program Organizers: David Restrepo, University of Texas at San Antonio; Steven Naleway, University of Utah; Jing Du, Pennsylvania State University; Ning Zhang, University of Alabama

Wednesday PM March 17, 2021

Session Chairs: Jing Du, Penn State University; Ning Zhang, The University of

Alabama

2:00 PM Invited Cancer Testbed for Breast and Prostate Cancer Bone Metastasis: Kalpana Katti¹; Haneesh Jasuja¹; Sumanta Kar¹; Dinesh Katti¹; ¹North Dakota State University

2:30 PM

Conformational Transition of G-Actin Subunits Controls the Deformation Behavior of Actin Filament: Sharad Jaswandkar¹; Kalpana Kattti¹; Dinesh Katti¹; ¹North Dakota State University

2:50 PM

Nanotechnology Enhanced Novel Bioresorbable Zn Alloy Implant for Short Bowel Syndrome Treatment: Jingke Liu¹; Zeyi Guan¹; Yuxin Zeng¹; Chase Linsley¹; James Dunn²; Bejamin Wu¹; Xiaochun Li¹; ¹University of California, Los Angeles; ²Stanford **University School of Medicine**

3:10 PM

Novel Zn-Fe-Si Alloy as Biodegradable Stent Material: Yuxin Zeng¹; Zeyi Guan¹; Jingke Liu¹; Xiaochun Li¹; ¹UCLA

3:30 PM Invited

Investigating the Remodeling of the Cellular and Collagen Tissue Structures of the Optic Nerve Head in Mouse Models of Glaucoma: Thao Nguyen¹; ¹Johns Hopkins University

4:00 PM Invited **Biomineralized Low-density Structural Materials**: *Ling Li*¹; ¹Virginia Polytechnic Institute



4:30 PM

Euplectella Aspergillum: Multiscale Structural Characterization, Quantification and Micromechanical Properties: *Swapnil Morankar*¹; Arun Singaravelu¹; Sridhar Niverty¹; Jason Williams²; Yash Mistry²; Clint Penick³; Dhruv Bhate²; Nikhilesh Chawla¹; ¹Purdue University; ²Arizona State University; ³Kennesaw State University

4:50 PM

Freeze Casting of Bioinspired Materials with Extrinsic Control Techniques: Steven *Naleway*¹; Isaac Nelson²; Tony Yin¹; Debora Lyn Porter¹; Josh Fernquist¹; Josh Alexander¹; Max Mroz¹; Paul Wadsworth¹; ¹University of Utah; ²Sandia National Lab

5:10 PM

Employing Electric Field in the Fabrication of Directionally Porous Ice-templated Ceramics: *Dipankar Ghosh*¹; Sashanka Akurati¹; Diego Terrones¹; Shizhi Qian¹; Bharath Gundrati¹; ¹Old Dominion University

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII — Structures and Modeling

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa **Technical Center**



WEDNESDAY PM

SI NE

Q

Wednesday PM March 17, 2021

Session Chairs: Juergen Eckert, Erich Schmid Inst of Materials Science; Katharine Flores, Washington University

2:00 PM Invited Brittle-to-Ductile Transition in Metallic Glasses: Jurgen Eckert¹; ¹Erich Schmid Institute of Materials Science

2:25 PM Invited **Correlated Disorder Order in a Model Binary Glass**: *Peter Derlet*¹; ¹Paul Scherrer Insitute

2:50 PM

Effect of Porosity on Fracture Behavior of Porous Bulk Metallic Glasses: Devashish *Rajpoot*¹; Parag Tandaiya¹; ¹Indian Institute of Technology Bombay

3:10 PM

Effective Quantification of Liquid Structure in Metallic Alloys and its Relation to Glass-Forming Ability: Porter Weeks¹; Katharine Flores¹; ¹Washington University in St Louis, Institute of Materials Science and Engineering

3:30 PM Invited Structural Relaxation and Mechanical Properties of Model Glass Systems at the **Micro-second Timescale**: *Peter Derlet*¹; Robert Maass²; ¹Paul Scherrer Insitute; ²University of Illinois at Urbana Champaign

3:55 PM

Emerging Fractal Potential Energy Landscape as the Origin of Activation Volume

in Metallic Glasses: Chaoyi Liu¹; Yue Fan¹; ¹University of Michigan

TMS WEBSITE

4:15 PM

Glass Forming Ability of the Cu-Zr Alloys: What Do We Learn from Molecular **Dynamics Simulation?**: *Mikhail Mendelev*¹; Yang Sun²; Feng Zhang¹; Cai-Zhuang Wang¹; Kai-Ming Ho¹; ¹Ames Laboratory; ²Columibia University

4:35 PM

Stress Breaks Universal Aging Behavior in a Metallic Glass: Amlan Das¹; Peter Derlet²; Chaoyang Liu¹; Eric Dufresne³; Robert Maass¹; ¹University of Illinois at Urbana Champaign; ²Paul Scherrer Institute; ³Argonne National Laboratory

4:55 PM

Local Structure of the Al-RE Marginal Metallic Glasses Studied by Molecular **Dynamics Simulation**: *Doguhan Sariturk*¹; Tolga Han Ulucan¹; Yunus Kalay¹; ¹Middle East Technical University

LIGHT METALS

Cast Shop Technology — Metal Treatment and Shape Casting

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Samuel Wagstaff, Oculatus

March 17, 2021 Wednesday PM

Session Chair: Filippos Patsiogiannis, Bridgnorth Aluminium



0

2:00 PM

Grain Refinement Efficiency: Rein Vainik¹; John Courtenay¹; Frode Lien¹; ¹MQP Ltd

2:20 PM

A Comparison of AA6060 Grain Structures Achieved Using AMG's TiBALAdvance™ and Alternative Al-Ti-B Grain Refiners via a 1D Upward Solidification Device: *Matthew Piper*¹; Shahid Akhtar²; Phil Enright³; ¹AMG Aluminum UK Limited; ²Hydro Aluminium Reseach Centre; ³NTec

2:40 PM

Mechanism of High Grain Refinement Effectiveness on New Grain Refiner "TiBAL Advance": Akihiro Minagawa¹; Matthew Piper²; ¹Uacj Corporation; ²AMG Aluminum

3:00 PM

Resonance for Contactless Ultrasonic Treatment in Direct Chill Casting: Catherine *Tonry*¹; Valdis Bojarevics¹; Georgi Djambazov¹; Koulis Pericleous¹; ¹Unviersity of Greenwich

3:20 PM

Ultrasonic Melt Treatment in a DC Casting Launder: The Role of Melt Processing **Temperature**: *Christopher Beckwith*¹; Tungky Subroto²; Koulis Pericleous¹; Georgi Djambazov¹; Dmitry Eskin²; lakovos Tzanakis³; ¹University of Greenwich; ²Brunel University London; ³Oxford Brookes University

3:40 PM

Residual Stress Prediction in the Casting Process of Automotive Powertrain **Components**: *Sina Kianfar*¹; Joshua Stroh¹; Nasim Bahramian¹; Dimitry G. Sediako¹; Anthony Lombardi²; Glenn Byczynski²; Philipp Mayr³; Mark Reid⁴; Anna Paradowska⁴; ¹University of British Columbia; ²Nemak Canada; ³Nemak Global; ⁴ANSTO

4:00 PM

Coupled Modeling of Misrun, Could Shut, Air Entrainment and Porosity for High **Pressure Die Casting Applications**: *Juergen Jakumeit*¹; Herfried Behnken¹; Romuald

Wednesday PM March 17, 2021

Laqua¹; Simon Mbewou²; Martin Fehlbier²; Julian Gänz³; Leonard Becker³; ¹Access E.V.; ²Foundry technic, University Kassel; ³Siemens Industry Software GmbH, DI SW STS CCM TO

4:20 PM

Study on the Mechanical Properties of Commercial Vehicle Wheel Through the Molten-Forged on the A356 Alloy with a Multi-cavity Fabrication Process: Min Seok Moon¹; Myeong Han Yoo¹; Kee Won Kim²; Joon Hyuk Song¹; Je Ha Oh¹; ¹Korea Institute of Carbon Convergence Technology; ²Rheoforge Co., Ltd.

4:40 PM Question and Answer Period

NUCLEAR MATERIALS

Ceramic Materials for Nuclear Energy Research and Applications — **Microstructure and Properties - Experiments and Modeling**

Sponsored by: TMS Extraction and Processing Division, TMS Structural Materials Division, TMS Light Metals Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Committee, TMS: Nuclear Materials Committee

Program Organizers: Xian-Ming Bai, Virginia Polytechnic Institute and State University; Yongfeng Zhang, University of Wisconsin-Madison; Larry Aagesen, Idaho National Laboratory; Vincenzo Rondinella, Jrc-Ec



Session Chairs: William Weber, University of Tennessee, Knoxville; Marat Khafizov, Ohio State University

2:00 PM Invited **Exotic Magneto-elastic Properties in Uranium Dioxide**: *Krzysztof Gofryk*¹; ¹Idaho National Laboratory

2:30 PM Invited Towards a Model of Coupled Irradiation and Corrosion: Amitava Banerjee¹; Aaron Kohnert¹; Edward Holby¹; Laurent Capolungo¹; *Blas Uberuaga*¹; ¹Los Alamos National Laboratory

3:00 PM

Impact of Dislocation Loops on Thermal Conductivity of CeO2: Marat Khafizov¹; Lingfeng He²; Miaomiao Jin²; David Hurley²; ¹Ohio State University; ²Idaho National Laboratory

3:20 PM

Microstructural Analysis and Micro-mechanical Testing on Xenon-irradiated Uranium Dioxide: Mack Cullison¹; Fei Teng²; David Fraser²; Boopathy Kombaiah²; Kun Mo³; Jie Lian⁴; Tianyi Chen¹; Fabiola Cappia²; ¹Oregon State University; ²Idaho National Laboratory; ³Argonne National Laboratory; ⁴Rensselaer Polytechnic Institute

3:40 PM Invited

Comprehensive Treatment of Thermal Transport Under Irradiation in ThO2: David Hurley¹; Marat Khafizov²; Cody Dennett¹; Amey Khanolkar¹; Zilong Hua¹; Lingfeng He¹; Jian Gan¹; Anter ElAzab³; Maneieha Salaken³; Chao Jiang¹; Miaomiao Jin¹; Ryan Deskins³; Bawane Kausubh¹; Chris Marianettii⁴; Matthew Mann⁵; ¹Idaho National Laboratory; ²Ohio State University; ³Purdue University; ⁴Columbia University; ⁵AFRL



TEM Characterization of Dislocation Loops in Ion-irradiated Single Crystal ThO₂: *Kaustubh Bawane*¹; Xiang Liu¹; Tiankai Yao¹; Marat Khafizov²; Aaron French³; Matthew Mann⁴; Lin Shao³; Jian Gan¹; David Hurley¹; Lingfeng He¹; ¹Idaho National Laboratory; ²Ohio State University; ³Texas A&M University; ⁴Air Force Research Laboratory

4:30 PM

Hydrothermal Corrosion of Silicon Carbide: *Jianqi Xi*¹; Dane Morgan¹; Izabela Szlufarska¹; ¹University of Wisconsin-Madison

4:50 PM

TMIST-3A Post-irradiation Examination: *Mark Lanza*¹; Walter Luscher¹; David Senor¹; Gary Hoggard²; ¹Pacific Northwest National Laboratory; ²Idaho National Laboratory

CHARACTERIZATION

Characterization of Materials through High Resolution Imaging — High Resolution Characterization of Materials with General Coherent Imaging Techniques

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Richard Sandberg, Brigham Young University; Ross Harder, Argonne National Laboratory; Xianghui Xiao, Brookhaven National Laboratory; Brian Abbey, La Trobe University; Saryu Fensin, Los Alamos National Laboratory;



Ana Diaz, Paul Scherrer Institut; Mathew Cherukara, Argonne National Laboratory

Wednesday PM March 17, 2021

Session Chair: Richard Sandberg, Brigham Young University

2:00 PM Keynote The Fourth is Strong in These Ones!: *Ian McNulty*¹; ¹MAX IV Laboratory

2:30 PM

X-ray Based Nanodiffraction to Study Strain in Materials for Nuclear Energy: *Ericmoore Jossou*¹; Mehmet Topsakal¹; Xiaojing Huang¹; Khalid Hattar²; Hanfei Yan¹; Yong Chu¹; Cheng Sun³; Lingfeng He³; Jian Gan³; Lynne Ecker¹; Simerjeet Gill¹; ¹Brookhaven National Laboratory; ²Sandia National Laboratories; ³Idaho National Laboratory

2:50 PM Invited

Imaging Phase Transitions of Quantum Materials with Bragg Coherent X-ray Diffraction: *Tadesse Assefa*¹; Yao Cao²; Jiecheng Diao³; Wonsuk Cha²; Ross Hardar²; Kim Kisslinger¹; Mark Dean¹; Genda Gu¹; John Tranquada¹; Ian Robinson¹; ¹Brookhaven National Laboratory; ²Argonne National Laboratory; ³University College London

3:20 PM

Mesoscale Defect Dynamics in the Bulk with Time-resolved Dark-field X-ray Microscopy: Leora Dresselhaus-Marais¹; ¹Lawrence Livermore National Laboratory

3:40 PM Invited

Laboratory and Synchrotron-based X-ray Tomographic Imaging during In Situ Loading of Materials: *Brian Patterson*¹; Lindsey Kuettner¹; Cindy Welch¹; Paul Welch¹; Axinte Ionita¹; Nikhilesh Chawla²; Xianghui Xiao³; ¹Los Alamos National

Laboratory; ²Arizona State University; ³Brookhaven National Laboratory

MOBILE-FRIENDL

WEDNESDAY PM

4:30 PM

Using the Rotation Vector Base Line Electron Back Scatter Diffraction (RVB-EBSD) Method to Characterize Single Crystal Cast Microstructures: Pascal Thome¹; Felicitas Scholz¹; Jan Frenzel¹; Gunther Eggeler¹; ¹Ruhr-University Bochum

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Advanced **Characterization Methods III**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

Wednesday PM March 17, 2021

Session Chairs: Jian Li, CanmetMATERIALS; Kim Jeongguk , Korea Railroad

4:10 PM

Magnetic Correlations and Time Fluctuations in Assemblies of Fe3O4 Nanoparticles Probed via X-rays: Karine Chesnel¹; ¹Brigham Young University

> TABLE NIENTS Q

2:00 PM

Nanotwinned Ni-Mo-W Alloys with Ultrahigh Strength and Localized Plasticity: *Gianna Valentino*¹; Jessica Krogstad²; Timothy Weihs¹; Kevin Hemker¹; ¹Johns Hopkins University; ²University of Illinois Urbana-Champaign

2:20 PM

FIB-SIMS in a Multi-Ion Source Plasma FIB: *Daniel Murray*¹; Xiaofei Pu¹; ¹Idaho National Lab

2:40 PM

In-situ Nanoscale Characterization of Phase Transformations in Materials **Undergoing Ultra-fast Heating and Cooling**: *Azin Akbari*¹; James Ranney¹; ¹ThermoFisherScientific

3:00 PM

A Study of the Absorption Edge of ZnO Thin Films Prepared by the Spray Pyrolysis **Method**: Shadia Ikhmayies; ¹

3:20 PM

Modeling Empirical Estimators for the 3D Particle Size, Distribution, and Expected Error from 2D Cross Sections of a Lognormal Distribution of Spherical Particles: Austin Gerlt¹; Amanda Criner²; Lee Semiatin²; Katelun Wertz²; Eric Payton²; ¹The Ohio State University; ²Air Force Research Lab

3:40 PM

Imaging Materials and their Evolution with High-Energy X-rays: Jonathan Almer¹; Peter Kenesei¹; Jun-Sang Park¹; Meimei Li¹; Paul Shade²; ¹Argonne National Laboratory; ²Air Force Research Laboratory



2:00 PM Invited

4:00 PM General Guideline of FIB Milling of Metal Alloys: *Jian Li*¹; ¹CanmetMATERIALS

4:20 PM Integrated, Table-top Instrumentation for High-temperature Thermal Property Measurements of Molten Salts: Haoxuan Yan¹; Federico Coppo¹; Uday Pal¹; ¹Boston University

ADDITIVE TECHNOLOGIES

Computational Techniques for Multi-Scale Modeling in Advanced Manufacturing — Modeling of Microstructural Evolution

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Extraction and Processing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, University of Alabama; Mei Li, Ford Motor Company; Alexandra Anderson, Gopher Resource; Srujan Rokkam, Advanced Cooling Technologies Inc

Wednesday PM March 17, 2021

Session Chair: Laurentiu Nastac, The University of Alabama

MOBILE-FRIEN



In Situ and Operando Synchrotron Experiments for Additive Manufacturing Model Validation: Peter Lee¹; Chu Lun Alex Leung¹; Yunhui Chen¹; Samuel Clark¹; Sebastian Marussi¹; Robert Atwood²; Martyn Jones³; Gavin Baxter³; ¹University College London; ²Diamond Light Source; ³Rolls-Royce plc

2:40 PM

Investigation of Powder Spattering in Laser Powder Bed Fusion through Multiphysics Modeling and High-speed Synchrotron X-ray Imaging: Xuxiao Li¹; Qilin Guo²; Zachary Young³; Fangzhou Li¹; Lianyi Chen²; Wenda Tan¹; ¹University of Utah; ²University of Wisconsin-Madison; ³Missouri University of Science and Technology

3:05 PM

Particle Resolved Simulation of Laser Powder-bed Fusion Including Metal **Evaporation and Vapor Plume Dynamics**: Juergen Jakumeit¹; Romuald Laqua¹; Gongyuan Zheng¹; Yuze Huang²; Samuel Clark²; Peter Lee²; ¹Access E.V.; ²University College London

3:30 PM

Phase-field Modeling of The Evolution Kinetics of Porous Structure During **Dealloying of Binary Alloys**: *jie li*¹; ¹The Hong Kong Polytechnic University

3:55 PM

Fluid Dynamics Effects on Microstructure Prediction in Single-Laser Tracks for Additive Manufacturing: Adrian Sabau¹; Lang Yuan²; Narendran Raghavan¹; Matthew Bement¹; John Turner¹; ¹Oak Ridge National Laboratory; ²University of South Carolina

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics — Phase Stability II



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

Wednesday PM March 17, 2021

Session Chair: Peter Galenko, Friedrich Schiller University Jena

2:00 PM

ThermodynamicStabilityoftheLightElementsDopinginSm(Fe,Co)₁₂**Compounds**: *Arkapol Saengdeejing*¹; Ying Chen¹; ¹Tohoku University

2:20 PM

First-principles Investigation of the Phase Structures and Stabilities in Mg-Zn Alloys: *Du Cheng*¹; Kang Wang¹; Bi-Cheng Zhou¹; ¹University of Virginia

2:40 PM

Stability and Phase Transition of Cristobalite in SiO₂: *Ying Chen*¹; Nguyen-Dung Tran¹; Hao Wang²; Masanori Kohyama³; Satoshi Kitaoka⁴; Tetsuo Mohri¹; ¹Tohoku University; ²Shanghai University; ³AIST; ⁴Japan Fine Ceramics Center (JFCC)

3:00 PM

Phase stability and Atomic Diffusion in fcc Fe-Ni Alloys: Interplay between



Magnetic and Chemical Degrees of Freedom: *Kangming LI*¹; Chu-Chun Fu¹; Maylise Nastar¹; ¹DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay

3:20 PM

Dislocation Formation Mechanism in Polycrystalline HCP Zr and Zr-2.5wt.%Nb Alloy: *Cong Dai*¹; Nana Ofori-Opoku¹; ¹Canadian Nuclear Laboratories

CORROSION

Environmental Degradation of Additively Manufactured Alloys — AM Materials and Aqueous Corrosion - Part I

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Additive Manufacturing Committee

Program Organizers: Kinga Unocic, Oak Ridge National Laboratory; Jenifer Locke, Ohio State University; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Xiaoyuan Lou, Auburn University; Brendy Rincon Troconis, University of Texas at San Antonio; Luke Brewer, University of Alabama

Wednesday PM March 17, 2021

Session Chairs: Jenifer S. Locke , The Ohio State University; Xiaoyuan Lou, Auburn University

2:00 PM

Comparing Corrosion of Alloys Made by Additive Manufacturing and Traditional

Methods: Sohrab Ghiasi¹; *Vineeth Kumar Gattu*²; William Ebert²; J Ernesto Indacochea¹; ¹University of Illinois at Chicago; ²Argonne National Laboratory

2:20 PM Anisotropic Electrochemical Response of Laser Powder Bed Additively Fused Ti6Al4V in Chloride Medium: *Sangram Mazumder*¹; Mangesh V. Pantawane¹; Yee-Hsien Ho¹; Narendra B. Dahotre¹; ¹University of North Texas

2:40 PM

Simulation of the Effect of Corrosion on the Mechanical Properties of Porous Mg Scaffolds Fabricated by Power Bed Laser Fusion for Biomedical Applications: M. Marvi-Mashhadi¹; Muzi Li²; Wahaaj Ali²; Carlos González³; *Javier Llorca*³; ¹Carlos III University; ²IMDEA Materials Institute; ³IMDEA Materials Institute & Technical University of Madrid

3:00 PM

Characterization of Corrosion Behavior in Additively Manufactured Al-6061 RAM Processed by Laser Powder Bed Fusion (L-PBF): *Hamidreza T-Sarraf*¹; Nikhilesh Chawla²; ¹Purdue University; ²Arizona State University

3:20 PM

Effect of Heat Treatment on the Stress Corrosion Cracking Behavior of an Additively Manufactured 7050 Aluminum Alloy Produced by Selective Laser Melting (SLM): *Kevin Chasse*¹; Crosby Owens¹; Rupesh Rajendran²; Preet Singh²; ¹Northrop Grumman Corporation; ²Georgia Institute of Technology

3:40 PM

Influence of Cold Spray Deposition Parameters on Pitting of AA2024: Ozymandias Agar¹; Luke Brewer¹; ¹University of Alabama



CORROSION

Environmentally Assisted Cracking: Theory and Practice — Stress Corrosion Cracking II

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Wednesday PM March 17, 2021

Session Chairs: James Burns , University of Virginia; Yiren Chen, Argonne National Lab

2:00 PM Invited Cracking Growth Behavior of Irradiated Stainless Steels in Light Water Reactors: *YirenChen*¹; BogdanAlexanderanu¹; Appajosula Rao²; ¹Argonne NationalLaboratory; ²Nuclear Regulatory Commission

2:40 PM

Stress Corrosion Cracking of TRIP Fe39Mn2OCo20Cr15Si5Al1 (at.%) High Entropy Alloy: *Pranshul Varshney*¹; Rajiv Mishra²; Nilesh Kumar¹; ¹University of Alabama Tusaloosa; ²University of North Texas

3:00 PM

An Alternate Approach to DCB Specimens for Determining Sulfide Stress Cracking Thresholds: Constant or Increasing Driving Force Specimens: *Carl Popelar*¹; W.

Hickey¹; James Sobotka¹; Julian Hallai²; Yifei Zeng²; ¹Southwest Research Institute;

²ExxonMobil Upstream Research Co

3:20 PM Invited The Effect of Loading Rate on Environment-assisted Cracking Behavior in Ti, Fe,

Al, and Ni-based Structural Alloys: James Burns¹; Zachary Harris¹; ¹University of Virginia

4:00 PM

Comparison of Surface Treatment Technologies for the Mitigation of Stress Corrosion Cracking in Al-Mg: Matthew McMahon¹; William Golumbfskie¹; Eric Dau²; ¹Naval Surface Warfare Center, Carderock Division; ²Vision Point Systems

4:20 PM

Understanding the Effect of Polarization on SCC Resistance and Crack Tip pH of AA6111-T8: Katrina Catledge¹; Mark Nichols²; Gerald Frankel¹; Jenifer Locke¹; ¹The Ohio State University; ²Ford Research and Advanced Engineering, Ford Motor Company

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Derivative Technologies for Dissimilar

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St.



WEDNESDAY PM

TABLE

Q

NTENTS

Petersburg Polytechnic University

Wednesday PM March 17, 2021

2:00 PM

An Analysis of Joint between AZ31 and DP590 Steel Created Using Friction-stir Assisted Scribe Technique: Metallurgical vs Mechanical Bonding: Shank Kulkarni¹; Hrishikesh Das¹; Daniel Tamayo¹; Piyush Upadhyay¹; Kyoo Sil Choi¹; Ayoub Soulami¹; ¹Pacific Northwest National Laboratory

2:20 PM

Oscillation Behavior of Dissimilar Aluminum/Steel Joints Realized by Ultrasound Enhanced Friction Stir Welding (USE-FSW): Marco Thoma¹; Andreas Gester¹; Guntram Wagner¹; ¹Chemnitz University of Technology

2:40 PM

Process Robustness of Friction Stir Dovetailing of AA7099 to Steel with In Situ AA6061 Interlayer Linking: Md Reza-E-Rabby¹; Timothy Roosendaal¹; Piyush Upadhyay¹; Nicole Overman¹; Joshua Silverstein¹; Martin McDonnell¹; Scott Whalen¹; ¹Pacific Northwest National Laboratory

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Additive Manufacturing / Rapid **Solidification**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Wednesday PM March 17, 2021

Session Chairs: Güven Kurtuldu, ETH Zürich; Ulrike Hecht, Access e.V.; Peter Voorhees, Northwestern University; Damien Tourret, IMDEA Materials

2:00 PM Invited Morphological Evolution during Solidification: Tiberiu Stan¹; Alexander Chadwick¹; Kate Elder¹; Xianghui Xiao²; *Peter Voorhees*¹; ¹Northwestern University; ²Brookhaven National Laboratory

2:30 PM

Quantification of the Extent of Disequilibrium at the Solid-liquid Interface during Additive Manufacturing: *Prabhakar Pal*¹; André Phillion¹; ¹McMaster University

2:50 PM

Grain Refinement Mechanisms of A6O61-RAM2 Metal Matrix Composite Alloys during Laser Powder Bed-fusion (LPB-F): *Chloe Johnson*¹; G. Becker¹; Kamel Fezzaa²; Jonah Klemm-Toole¹; Jeremy Iten³; Amy Clarke¹; ¹Colorado School of



Mines; ²Argonne National Laboratory; ³Elementum 3D

3:10 PM Invited In Situ Studies of Alloy Solidification Using Dynamic TEM: Joseph McKeown¹; ¹Lawrence Livermore National Laboratory

3:40 PM

Rapid Solidification of Polycrystalline Al-Cu with a Quantitative Phase Field Model and In-situ Imaging: *Tatu Pinomaa*¹; Joseph McKeown²; Anssi Laukkanen¹; Jörg Wiezorek³; Nikolas Provatas⁴; ¹VTT Technical Research Centre of Finland; ²Lawrence Livermore National Laboratory; ³University of Pittsburgh; ⁴McGill University

4:00 PM

Numerical Model of Al-33wt%Cu Eutectic Growth during Impulse Atomization: Jonas Valloton¹; Abdoul-Aziz Bogno¹; Michel Rappaz²; Hani Henein¹; ¹University of Alberta; ²Ecole Polytechnique Fédérale de Lausanne

NANOSTRUCTURED MATERIALS

Functional Nanomaterials: Functional Low-dimensional Materials (OD, 1D, 2D) Driving Innovations in Electronics, Energy, Sensors, and Environmental Engineering and Science 2021 — 2D Materials & Nanostructures

Sponsored by: TMS Functional Materials Division, TMS: Nanomaterials Committee

Program Organizers: Jiyoung Chang, University of Utah; Michael Cai Wang, University of South Florida; Sarah Zhong, University of South Florida; Sun Choi, Korea Institute of Science and Technology; Pei Dong, George Mason University

TMS

Wednesday PM March 17, 2021

MOBILE-FRIEND

CONTENTS

FABLE OF

Session Chairs: Michael Wang, University of South Florida; Sarah Zhong, University of South Florida

2:00 PM Invited **2D Thermoelectric Devices**: *Xian Zhang*¹; ¹Stevens Institute of Technology

2:25 PM Invited Intrinsic and Interfacial Fatigue of Graphene: Tobin Filleter¹; ¹University of Toronto

2:50 PM Invited Janus Monolayer-Induced Abnormal Mechanical and Optical Properties in 2D Heterostructures: Shengxi Huang¹; ¹The Pennsylvania State University

3:15 PM

PhotoresponseCharacterizationofAuNanorodsCoatedPtSe,:*TatsuyaNakazawa*¹; Shinichi Kato²; Donghyun Kim¹; Jwa-Min Nam²; Hyungjun Kim¹; ¹Yonsei University; ²Seoul National University

3:35 PM Invited

Rapid Water Harvesting and Non-thermal Drying in Humid Air by N-doped Graphene Micro-Pads: Yiyang Wan¹; Yong Gao²; *Zhenhai Xia*¹; ¹University of North Texas; ²Northewstern Polytechnical University

4:00 PM Invited Two-dimensional Transition Metal Dichalcogenides for Optoelectronics and **Chemiresistive Applications**: *Jungwook Choi*¹; ¹Yeungnam University



WEDNESDAY PM

4:25 PM

WSe, Growth on Hafnium Zirconium Oxide by Molecular Beam Deposition: The Effect of Growth Conditions on the Substrate Properties: Maria Gabriela Sales¹; Shelby Fields²; Samantha Jaszewski²; Sean Smith³; Riley Christopher⁴; Nikhil Shukla⁴; Jon Ihlefeld²; Stephen McDonnell²; ¹University of Virginia; ²Department of Materials Science and Engineering, University of Virginia; ³Materials Science and Engineering Center, Sandia National Laboratories; ⁴Department of Electrical and Computer Engineering, University of Virginia

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Functional Heterostructured Materials

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of **Sciences**

March 17, 2021 Wednesday PM

Session Chairs: Peter Anderson, Ohio State University; Jagannathan Rajagopalan, Arizona State University; Anding Wang, City University of Hong KOng



2:00 PM Invited

Shape Memory Alloys: Using Heterostructure-induced Defects to Train Thermomechanical Response: *Peter Anderson*¹; Harshad Paranjape²; Sivom Manchiraju³; Michael Mills¹; ¹Ohio State University; ²Confluent Medical Technologies; ³Ansys, Inc.

2:25 PM

High Strength and Low Coercivity Cobalt with Three-dimensional Planar Defects Introduced by Heterogeneous Coherent Interface: Jian Song¹; Guisen Liu¹; Y. Liu¹; J. Wang²; X. Zhang³; ¹Shanghai Jiao Tong University; ²University of Nebraska-Lincoln; ³Purdue University

2:45 PM

Analysis of Inertially Dampened Structure in High Strain Rate Impacts: Trenin *Bayless*¹; Jerome Downey¹; ¹Montana Technological University

3:05 PM

Interface Engineered Tungsten Based Nanocomposites and Nanofoams for Harsh **Environments**: *Daniel Kiener*¹; Mingyue Zhao¹; Inas Issa¹; Michael Wurmshuber¹; ¹University of Leoben

3:25 PM

Hydrogen Charging Behavior of Gradient Structured High-Mn Steels: Jung Gi Kim¹; Hyun Joo Seo²; Jeong Min Park²; Seung Mi Baek²; Auezhan Amanov³; Chong Soo Lee²; Hyoung Seop Kim²; ¹Gyeongsang National University; ²Pohang University of Science and Technology; ³Sun Moon University

3:45 PM

Effects of Constituent Properties on Propagating Stress Waves in Multiphase



WEDNESDAY PM

ONTENTS

TABLE OF

Composites: Avery Samuel¹; Irene Beyerlein¹; Frank Zok¹; ¹University Of California, Santa Barbara

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Structures and **Mechanical Properties II**

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Wednesday PM March 17, 2021

Session Chairs: Saryu Fensin, Los Alamos National Laboratory; Nan Li, Los Alamos National Laboratory

2:00 PM Invited

Dynamic Properties of a High Entropy Alloy -- FeCrMnNi: Michelle Hawkins¹; Robert Hixson²; Jonathan Gigax²; Nan Li²; Sarah Thomas¹; *Saryu Fensin*²; ¹Mission Support and Test Services, LLC; ²Los Alamos National Laboratory

2:20 PM

Effect of Cooling Rate on the High Strain Rate Deformation of Dual-phase High

EntropyAlloy: Samrat Tamuly¹; Saurabh Dixit¹; V Parameswaran¹; Prasenjit Khanikar¹;

¹Indian Institute of Technology Guwahati

2:40 PM Mechanical and Elastic Behavior as Well as Microstructural Response of NbTaTiV and NbTaTiVZr as a Function of Strain Rate: Mathew Hayne¹; Saryu Fensin¹; Tarik Saleh¹; Chanho Lee²; Peter Liaw²; ¹Los Alamos National Laboratory; ²The University of Tennessee

3:00 PM

Deformation Mechanism and Microstructural Evolution in Al₀₄CoCrFeNi High **Entropy Alloy**: Anumat Sittiho¹; Jadzia Graves¹; Sanjit Bhowmick²; Indrajit Charit¹; Rajiv Mishra³; ¹University of Idaho; ²Bruker; ³University of North Texas

3:20 PM

On the Phase Stability, Mechanical Properties, and Deformation Mechanisms of the Equiatomic CrFeNi Medium-entropy Alloy: Mike Schneider¹; Guillaume Laplanche¹; ¹Ruhr-Universitat Bochum

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling - Modeling and Machine Learning

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University;



Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Wednesday PM March 17, 2021

Session Chairs: Yu Zhong, Worcester Polytechnic Institute; Jia Li, Hunan University

2:00 PM Invited The Application of High-throughput Calculations in High Entropy Alloys : Yu Zhong¹; ¹Worcester Polytechnic Institute

2:25 PM Invited Extrapolation of Machine Learning Models for Designing Multi-principal Element Alloys: James Saal¹; Chris Borg¹; Clara Nyby¹; Bryce Meredig¹; ¹Citrine Informatics

2:50 PM

Machine Learning Enabled Prediction of Stacking Fault Energies in Concentrated Alloys: Gaurav Arora¹; Anus Manzoor¹; Dilpuneet Aidhy¹; ¹University of Wyoming

3:10 PM Invited Optimalizing Properties of High Entropy Alloy by Machine Learning and Multiscale **Simulations**: *Jia Li*¹; Yang Chen¹; Qihong Fang¹; ¹Hunan University

3:35 PM

Accelerated Exploration of Refractory Multi-principal Element Alloys by Machine Learning: Carolina Frey¹; Christopher Borg²; James Saal³; Bryce Meredig³; Daniel Miracle⁴; Tresa Pollock¹; ¹University of California, Santa Barbara; ²Citrine Informatics ; ³Citrine Informatics; ⁴Air Force Research Laboratory



3:55 PM Ab Initio Modeling on the Elastic Properties of Al-Co-Cr-Fe-Ni High Entropy Alloys: A Case Study with FCC Phase: Songge Yang¹; Jize Zhang¹; Yu Zhong¹; ¹Worcester Polytechnic Institute

MATERIALS PROCESSING

High Temperature Electrochemistry IV — Session V

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Guy Fredrickson, Idaho National Laboratory

Wednesday PM March 17, 2021

Session Chair: Hojong Kim, The Pennsylvania State University

2:00 PM

Advances in Solid Oxide Membrane Based Electrolysis for Solar-grade Silicon Deposition: *Michelle Sugimoto*¹; Haoxuan Yan¹; Federico Coppo¹; Adam Powell²; Uday Pal¹; ¹Boston University; ²Worchester Polytechnic Institute

2:30 PM

Feasibility of Potentiometry for Monitoring Activity of GdCl3 in Molten LiCl-KCl Salt: *Guoping Cao*¹; Steven Herrmann¹; Guy Fredrickson¹; Robert Hoover¹; Kevin



Tolman¹; ¹Idaho National Laboratory

3:00 PM First-principles Molecular Dynamics and CALPHAD Modeling of the CaF2-MgF2-SiO2 Molten Salt System: *Yifan Zhang*¹; Uday Pal²; Adam Powell¹; Michael Gao³; Yu Zhong¹; ¹Worcester Polytechnic Institute; ²Boston University; ³National Energy Technology Laboratory

MATERIALS DESIGN

Hume-Rothery Symposium: Accelerated Measurements and Predictions of Thermodynamics and Kinetics for Materials Design and Discovery — Session VI

Sponsored by: TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Wei Xiong, University of Pittsburgh; Shuanglin Chen, CompuTherm LLC; Wei Chen, Illinois Institute of Technology; James Saal, Citrine Informatics; Greta Lindwall, KTH Royal Institute of Technology

Wednesday PM March 17, 2021

Session Chair: Qiaofu Zhang, QuesTek Innovations LLC

2:00 PM Invited Integrated Predictive Materials Science: Filling the ICME Pipeline: John Allison¹; ¹University of Michigan

2:40 PM Invited

Phonon Anharmonicity Causes the Large Thermal Expansion of NaBr: Brent

*Fultz*¹; Yang Shen¹; Claire Saunders¹; Camille Bernal¹; Michael Manley²; ¹California

Institute of Technology; ²Oak Ridge National Laboratory

3:20 PM Invited Multi-cell Monte Carlo Method for Phase Prediction: Maryam Ghazisaeidi¹; You Rao¹; Edwin Antillon²; changning Niu³; Wolfgang Windl¹; ¹Ohio State University; ²Naval Research Lab; ³QuesTek Innovations LLC

4:00 PM Invited Insights from a Comprehensive Assessment of Diffusion Coefficients of 20 Binary Systems and a Comprehensive Diffusion Mobility Database for Magnesium Alloys: Wei Zhong¹; Qiaofu Zhang²; Ji-Cheng Zhao¹; ¹University of Maryland; ²QuesTek Innovations LLC

LIGHT METALS

Magnesium Technology 2021 — Alloying & Processing / Primary Production

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Petra Maier, University of Applied Sciences Stralsund; J. Brian Jordon, University of Alabama; Neale Neelameggham, IND LLC

Wednesday PM March 17, 2021

Session Chairs: Vineet Joshi, Pacific Northwest National Laboratory; Joshua Caris, Terves, LLC



WEDNESDAY PM

TABLE

Q

ONTENTS

2:00 PM

Absorbable Wire Radiopacity: Influence of Composition and Size on X-ray **Visibility**: *Adam Griebel*¹; Aubrey Ehle²; Jeremy Schaffer¹; ¹Fort Wayne Metals; ²Indiana University School of Medicine

2:20 PM

Magnesium and Magnesium Alloy Powder Processing Towards the Development of Near Shape Structural Materials: Steven Johnson¹; Dylan Goncalves¹; ¹Central **Connecticut State University**

2:40 PM

Effect of Processing Parameters on the Microstructure and Mechanical Behavior of Additively Manufactured WE43 Mg Alloy: Leila Sorkhi¹; Joshua Hammell¹; Grant Crawford¹; ¹South Dakota School of Mines & Tecchnogy

3:00 PM

Effects of Hot Isostatic Pressing on the Microstructure and Properties of Mg-Gd-Y-Zn Alloys: Janet Meier¹; Joshua Caris²; Alan Luo¹; ¹Ohio State University; ²Terves LLC

3:20 PM

Low-cost Magnesium Primary Production Using Gravity-driven Multiple Effect Thermal System (G-METS) Distillation: Madison Rutherford¹; Armaghan Ehsani Telgerafchi¹; Gabriel Espinosa¹; Adam Powell¹; David Dussault²; ¹Worcester Polytechnic Institute; ²Elemental Beverage

3:40 PM

Efficient Low-cost Gravity-driven Multiple Effect Thermal System (G-METS) **Distillation of Magnesium**: Armaghan Telgerafchi¹; Gabriel Espinosa¹; Madison Rutherford¹; Adam Powell¹; David Dussault²; ¹Worcester Polytechnic Institute; ²Elemental Beverage Company



2:00 PM Invited **Development and Management of Industrial Park for Chinese Electroplating** Industry: Yong Shi¹; Cuiping Huang¹; *Zhibo Huang*²; Jiann-Yang Hwang³; ¹Futianbao Environmental Protection, Ltd; ²Futianbo Environment Protection Technology, Ltd; ³Michigan Technological University

4:00 PM Industrial Practice of Extracting Magnesium from Serpentine: Huimin Lu¹; Neale Neelameggham²; ¹Beijing Ofikintai Technology Co., Ltd.; ²IND LLC

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Wastewater Treatment

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao, University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology Company Ltd.; Shadia Ikhmayies

Wednesday PM March 17, 2021

Session Chairs: Jinjing Luo, Xiamen University; Jiann-Yang Hwang, Michigan **Technological University**

CONTENTS TABLE OF





WEDNESDAY PM

2:20 PM Invited Mercury Removal by Bio-chars with Plasma Surface Modification: Jinjing Luo¹; ¹Xiamen University

2:40 PM Invited

Electroplating Wastewater Treatment in China: Zhibo Huang¹; Jiann-Yang Hwang²; Cuiping Huang¹; Yong Shi¹; ¹Futianbo Environment Protection Technology, Ltd; ²Michigan Technological University

3:00 PM Invited

Effects of Ozone on COD Reduction in Electroplating Wastewater: Yahui Sun¹; Jiann-Yang Hwang²; Lili Xi¹; Zhixing Fu¹; Fujiu Nian¹; Yang Yang¹; Xin Chen¹; ¹Futianbo Environment Protection Technology, Ltd; ²Michigan Technological University

3:20 PM

Extraction of Cerium from Catalyst of Waste Automobile Exhaust Gas Purifier: Chen Ailiang¹; *Guanwen Luo*¹; Mao Jiale¹; Lu Sujun²; Ma Yutian²; Du Zuojuan¹; Chen Shengli²; Pan Yujun¹; Qiao Jinxi¹; Bowen Li³; ¹Central South University; ²State Key Laboratory of Nickel and Cobalt Resources Comprehensive Utilization; ³Michigan Technological University

3:40 PM Invited

A New Electroplating Wastewater Treatment Process Using Electric Lime and Vacuum Filtration: Zhixing Fu¹; Jiann-Yang Hwang²; Yahui Sun¹; Yang Yang¹; Fujiu Nian¹; Lili Xi¹; Zhibo Huang¹; ¹Futianbo Environment Protection Technology, Ltd; ²Michigan Technological University

4:00 PM



Environmental protection technology; ²Michigan Technological University

4:20 PM Invited

Oxidation of Cyanide and Simultaneous Copper Electrodeposition from Electroplating Wastewater in an Electrochemical Reactor: Yang Yang¹; Fujiu Nian¹; Dong Xu¹; Yahui Sun¹; Jiann-Yang Hwang²; Peiyu Qiao¹; Zhixing Fu¹; Lili Xi¹; ¹Futianbo Environment Protection Technology, Ltd; ²Michigan Technological University

4:40 PM Invited

Treatment of Electroless Nickel Plating Wastewater by Ozone Oxidation: Lili Xi¹; Yahui Sun¹; Jiann-Yang Hwang²; Fujiu Nian¹; Zhixing Fu¹; Yang Yang¹; Cuiping Huang¹; ¹Futianbo Environment Protection Technology, Ltd; ²Michigan Technological University

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and Beyond — Refractory Alloys: Processing and Properties of Novel Materials

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University



WEDNESDAY PM

2:00 PM Invited

High-temperature, Thermally-cyclable, Reaction-formed, Co-continuous **Refractory Metal/Ceramic Composites for Extreme Environments**: *Kenneth* Sandhage¹; Yujie Wang¹; Priyatham Tumurugoti¹; Camilla McCormack¹; Alex Strayer¹; Adam Caldwell¹; Gregory Scofield¹; Zhenhui Chen¹; Raheleh Rahimi¹; Thuan Nguyen¹; Saeed Bagherzadeh¹; Kevin Trumble¹; Michael Sangid¹; Grigorios Itskos¹; Mario Caccia¹; ¹Purdue University

2:30 PM

ICME-guided Design of Novel Metal Matrix Composites for Extreme Environments: David Linder¹; *Martin Walbrühl*¹; Qiaofu Zhang²; ¹QuesTek Europe AB; ²QuesTek Innovations

2:50 PM Invited

Advanced Refractory Alloys for Use at Temperatures above 1273K: Oleg Senkov¹; Satish Rao¹; Todd Butler¹; Tinuade Daboiku¹; Eric Payton¹; ¹Air Force Research Laboratory

3:20 PM

Oxidation-resistant, Thermally-cyclable, Robust Oxide/Metal Composite Materials for Concentrated Solar Power: Camilla McCormack¹; Mario Caccia¹; Thuan Dinh Nguyen¹; Gregory Scofield¹; Grigorios Itskos¹; Michael Sangid; Kenneth Sandhage¹; ¹Purdue University

3:40 PM

Hot Isostatic Pressing of Niobium-based Refractory Alloy Powders: Calvin Mikler¹; Brian Welk¹; Benjamin Georgin¹; Todd Butler²; Noah Philips³; Hamish Fraser¹; ¹The Ohio State University; ²Air Force Research Laboratory; ³ATI Specialty Alloys and

TMS



A Review of Plastic Flow and Microstructure Evolution at Elevated-temperatures

in Unalloyed Niobium: *Emily Brady*¹; Eric Taleff¹; ¹University of Texas at Austin

4:20 PM

4:00 PM

Effect of Alloy Composition on the Microstructure of Developmental Iridium Alloys: Noah Kohlhorst¹; Glenn Romanoski²; Govindarajan Muralidharan²; Roger Miller²; Ji-Cheng Zhao³; ¹Ohio State Univerity; ²Oak Ridge National Laboratory (ORNL); ³University of Maryland, Department of Materials Science and Engineering

4:40 PM

Kinetics of Grain Boundary Segregation in an Ir Alloy*: Dean Pierce¹; Govindarajan Muralidharan¹; Jon Poplawsky¹; George Ulrich¹; ¹Oak Ridge National Laboratory

MATERIALS PROCESSING

Materials Processing Fundamentals — Metal Processing and Manufacturing

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Process Technology and Modeling Committee

Program Organizers: Jonghyun Lee, Iowa State University; Samuel Wagstaff, Oculatus; Alexandra Anderson, Gopher Resource; Fiseha Tesfaye, Abo Akademi University; Guillaume Lambotte, Boston Metal; Antoine Allanore, Massachusetts Institute of Technology



WEDNESDAY PM

NTENTS

Q

Wednesday PM March 17, 2021

Session Chairs: Allie Anderson, Gopher Resource; Yunbo Wang, Caterpillar Inc.

2:00 PM

Effect of Dissolution of Titanium Ions on Ti Alloys Electrodeposition from EMIC-AlCl, Ionic Liquid at Low Temperature: Pravin Shinde¹; Ramana Reddy¹; ¹The University Of Alabama

2:20 PM

Cylindrical and Planar Magnetron Sputtering for Microstructural Control: Adie *Alwen*¹; Alina Garcia Taormina¹; A.M. Hodge¹; ¹University of Southern California

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Creep, Fatigue, and Fracture

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee

Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory



CONTENTS

TABLE

P

2:00 PM Invited Multiscale Modeling of Creep and Transient Conditions in Steels: Application to HT9 Steel Alloy: Mariyappan Arul Kumar¹; Aaron Tallman¹; Christopher Matthews¹; Laurent Capolungo¹; ¹Los Alamos National Laboratory

2:30 PM

Creep Crack Growth Behaviour of Austenitic Stainless Steels Alloy 709 and 316H: Suyang Yu¹; Jin Yan¹; Hangyue Li¹; Afsaneh Rabiei²; Paul Bowen¹; ¹University of Birmingham; ²North Carolina State University

2:50 PM

Stress Corrosion Cracking Resistance of FeCrAl Alloys in Light Water Reactor Environments: Raul Rebak¹; Liang Yin¹; Andrew Hoffman¹; ¹GE Global Research

3:10 PM

Enabling In-situ Crack Growth Testing and Monitoring in VTR Cartridge Loop **Environments**: *Samuel Briggs*¹; Peter Beck¹; Dustin Mangus¹; Jake Quincey¹; Andrew Brittan¹; George Young¹; Guillaume Mignot¹; Julie Tucker¹; ¹Oregon State University

3:30 PM Invited

In-situ Scanning Electron Microscopic Observation of Creep and Creep-fatigue of Alloy 709: Amrita Lall¹; Rengen Ding²; Paul Bowen²; Afsaneh Rabiei¹; ¹North Carolina State University; ²University of Birmingham

4:00 PM

Mechanical Characterization of Neutron Irradiated HT-9 Heats (ORNL, LANL and EBR II) at LWR and Fast Reactor Relevant Temperatures: Ramprashad *Prabhakaran*¹; Mychailo Toloczko¹; Kumar Sridharan²; ¹Pacific Northwest National Laboratory; ²University of Wisconsin-Madison



WEDNESDAY PM

4:20 PM

Burst Behavior of Accident Tolerant Fuel Cladding Concepts under Simulated Loss-of-coolant Conditions: Samuel Bell¹; Bruce Pint¹; Ken Kane¹; ¹Oak Ridge National Laboratory

4:40 PM

C-ring Compression of SiC-SiC Cladding at 1200°C with In-situ X-ray Computed Micro-tomography: Dong Liu¹; Jon Ell²; Guanjie Yuan¹; Peng Xu³; Roger Lu⁴; Edward Lahoda⁴; Harold Barnard²; Dula Parkinson²; Robert Ritchie²; ¹University of Bristol; ²Lawrence Berkeley National Laboratory; ³Idaho National Laboratory; ⁴Westinghouse Electric Company

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ **Experiments and Modeling – Session VI**

Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

Wednesday PM March 17, 2021



2:00 PM

Synchrotron X-ray Studies of Deformation and Failure in Cold Spray Composites: Lewei He¹; Darren Pagan¹; Qi An¹; Aaron Nardi²; *Mostafa Hassani*¹; ¹Cornell University; ²U.S. Army Research Laboratory

2:20 PM

Metal Foams: Linking Dynamic CT Results to Simulation and Modeling: Luke Hunter¹; Wesley De Boever²; Martina Humbert³; Andreas Griesser³; ¹Tescan USA, Inc; ²TESCAN XRE; ³Math2Market

2:40 PM

Non-destructive Inspection of Contaminated Epoxy Plates Using Propagating Acoustic Waves: Isabel McBrayer¹; Fady Barsoum²; ¹Embry-Riddle Aeronautical University; ²Embry-Riddle Aeronautical University

3:00 PM

Rhodium and Cobalt Oxidation: A Nanoscale Study by In-situ and in Operando Atom Probe Tomography: Sten LAMBEETS¹; Norbert Kruse²; Daniel Perea¹; ¹Pacific Northwest National Laboratory; ²Washington State University

3:40 PM

Experimental Measurements of Anisotropic Mechanical Behavior of -HMX Crystals: Ayotomi Olokun1; Abhijeet Dhiman1; Vikas Tomar1; 1Purdue University

MATERIALS PROCESSING



MOBILE-FRIEND

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — **Pyrometallurgy II**

Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

Wednesday PM March 17, 2021

2:00 PM

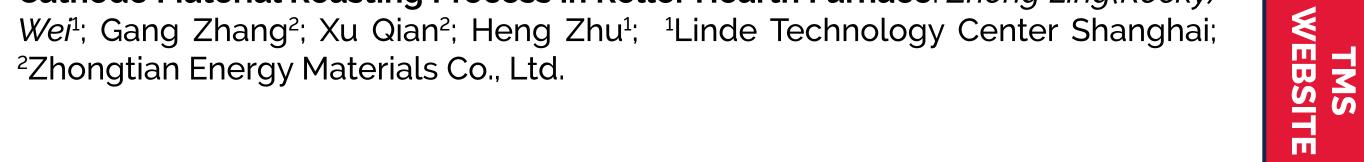
A Novel Process to Reduce SO, Emissions during Electric Furnace Smelting of Sulphides: David Tisdale¹; Sari Muinonen¹; Michael Molinski¹; Arthur Stokreef¹; ¹Glencore Sudbury Integrated Nickel Operations

2:20 PM

Influence of the Cemented Carbides Composition on the Disintegration in Liquid Zinc: Tamara Ebner¹; Stefan Luidold¹; Christoph Czettl²; Christian Storf²; ¹Montanuniversitaet Leoben; ²CERATIZIT Austria GmbH

2:40 PM

Study on CFD and Oxygen Lance Injection Technology of High Nickel Ternary Cathode Material Roasting Process in Roller Hearth Furnace: Zhong Ling(Rocky)



3:00 PM Real-time Fe End-point Determination at Sudbury INO Smelter Finishing Converter Using Thermodynamic Process Simulation: *Tanai Marin-Alvarado*¹; Brett MacKinnon¹; Arina Moraes¹; Kurt Westhaver¹; Phil Nelson¹; Nicolas Lazare¹; Vince McIver²; Sari Muinonen²; ¹XPS Expert Process Solutions; ²Sudbury Integrated Nickel Operations

ELECTRONIC MATERIALS

Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XX — Properties and Microstructures of Electronic Materials

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Hiroshi Nishikawa, Osaka University; Shih-kang Lin, National Cheng Kung University; Chao-Hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jaeho Lee, Hongik University; Zhi-Quan Liu, Shenzhen Institutes of Advanced Technology; Ming-Tzer Lin, National Chung Hsing University; Dajian Li, Karlsruhe Institute of Technology; Yu Zhong, Worcester Polytechnic Institute; Yee-wen Yen, National Taiwan University of Science and Technology; A.S.Md Abdul Haseeb, University of Malaya; Ligang Zhang, Central South University; Sehoon Yoo, KITECH; Vesa Vuorinen, Aalto University; Yu-chen Liu, National Cheng Kung University

Wednesday PM March 17, 2021



Session Chairs: A.S. Md. Abdul Haseeb, University of Malaya; Chih-Ming Chen, National Chung Hsing University

2:00 PM Keynote Effect of Initial Volume Ratio and Reflow Temperature on the Microstructure of SnBiAg-SAC Mixed Solder Joints: *Eric Cotts*¹; Faramarz Hadian¹; Randy Owen¹; Mohammed Genanu¹; ¹Binghamton University

2:40 PM

Effect of Low Bi Content on Mechanical Property of Sn-Bi-Zn Alloy before and after Thermal Aging: *Hiroshi Nishikawa*¹; Shiqi Zhou¹; Chih-han Yang²; Yu-An Shen²; Shih-kang Lin²; ¹Osaka University; ²National Cheng Kung University

3:00 PM

High-throughput Calculations for Sn-Bi-Ag and Sn-Bi-Ag-In Low-temperature Lead-free Solders: *Chih-Han Yang*¹; Yuki Hirata²; Hiroshi Nishikawa²; Shih-kang Lin¹; ¹National Cheng Kung University; ²Osaka University

3:20 PM

Solid-liquid Interfacial Reaction between Cu and In-48Sn Alloy: *F. L. Chang*¹; C. Robert Kao¹; H. T. Hung¹; S. Y. Lin¹; ¹National Taiwan University

3:40 PM

Using Machine Learning to Predict Hardness of Sn-based Alloys: *Yu-chen Liu*¹; Chih-han Yang¹; Hannah Carillo¹; Chuan-cheng Lin¹; Shih-kang Lin¹; ¹National Cheng Kung University

Phase Transformations and Microstructural Evolution — High Entropy Alloys



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Wednesday PM March 17, 2021

Session Chair: Bharat Gwalani, Pacific Northwest National Laboratory

2:00 PM

Microstructutal Evolution of Metals at High Temperature Revealed by In-situ **Neutron and Synchrotron X-ray Diffraction**: *Klaus-Dieter Liss*¹; ¹Guangdong Technion - Israel Institute of Technology (GTIIT)

2:20 PM

Atomistic Modeling of the Effects of Precipitates in Phase Stability of Fe-Ni Based Alloys: Eva Zarkadoula¹; Ying Yang¹; Albina Borisevic¹; Easo George¹; ¹Oak Ridge National Laboratory

2:40 PM

Microstructural Characterization of As-cast Al₂₇CrFeMnV, Al₂₇CrFeTiV, and Al, CrMnTiV High Entropy Alloys: Keith Knipling¹; Patrick Callahan¹; David Beaudry²;

ONTENTS

TABLE OF

Richard Michi³; ¹U.S. Naval Research Laboratory; ²Johns Hopkins University; ³Oak Ridge National Laboratory

3:00 PM

Comparison of Low Temperature Oxidation Behavior of Pure W and MoNbTaW **Thin Films**: *Robert Quammen*¹; Paul F. Rottmann¹; ¹University of Kentucky

3:20 PM

Hydrogen-induced Microstructural Transformations in an FeMnCoCr Highentropy Alloy: Maria Ronchi¹; Haoxue Yan¹; Shaolou Wei¹; C. Tasan¹; ¹Massachusetts Institute of Technology

3:40 PM

Stacking Fault Energy in Metastable Alloys: Mulaine Shih¹; Maryam Ghazisaeidi¹; ¹Ohio State University

MATERIALS PROCESSING

Rare Metal Extraction & Processing – V, Ce, Mo, Cr, Fe

Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

Wednesday PM March 17, 2021



2:00 PM Study on the Enhancement of Iron Removal in the Becher Aeration by a Novel Tubular Reactor: *Lei Zhou*¹; Qiuyue Zhao¹; Mingzhao Zheng¹; Zimu Zhang¹; Guozhi Lv¹; Tingan Zhang¹; ¹Northeastern University

ELECTRONIC MATERIALS

Recent Advances in Functional Materials and 2D/3D Processing for Sensors, Energy Storage, and Electronic Applications — Functional Materials and Printed Electronic Devices

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Pooran Joshi, Oak Ridge National Laboratory; Rahul Panat, Carnegie Mellon University; Ravindra Nuggehalli, New Jersey Institute of Technology; Tolga Aytug, Oak Ridge National Laboratory; Yong Lin Kong, University of Utah; Konstantinos Sierros, West Virginia University

Wednesday PM March 17, 2021

Session Chairs: Pooran Joshi, Oak Ridge National Laboratory; Ravindra Nuggehalli, New Jersey Institute of Technology; Konstantinos Sierros, West Virginia University

2:00 PM Invited 3D Printed Passive Sensors: An Overview: Vishal Mehta¹; Nuggehalli Ravindra²;



¹Ohio Northern University; ²New Jersey Institute of Technology

2:25 PM Invited

Direct Metal Contacts Printing on 4H-SiC for Radiation Detection: *Neil Taylor*¹; Yongchao Yu²; Mihee Ji²; Nora Dianne Ezell²; Pooran Joshi²; Lei Raymond Cao³; ¹Oak Ridge National Laboratory; The Ohio State University; ²Oak Ridge National Laboratory; ³The Ohio State University

2:50 PM

Modeling of Rheological Properties of Metal Nanoparticle Conductive Inks for Printed Electronics: *Patrick Dzisah*¹; Nuggehalli Ravindra¹; ¹New Jersey Institute of Technology

3:10 PM

High Strength Nanotwinned Copper Foils for Current Collectors in Lithium Ion Battery: *Fu Chian Chen*¹; Chen Chih¹; ¹National Chiao Tung University

3:30 PM Invited Advancing Multiscale 3D Printing of Bioelectronics with Soft Matter Physics: *Yong Lin Kong*¹; ¹University of Utah

3:55 PM Invited Nanostructured Thin Film Enabled Thermal Emission Based Passive Sensing for Extreme Environment Applications with Optical Fibers: *Paul Ohodnicki*¹; Sheng Shen²; Henry Du³; ¹University of Pittsburgh; ²Carnegie Mellon University; ³Stevens Institute of Technology

ENERGY & ENVIRONMENT

Recycling and Sustainability for Emerging Technologies and Strategic

TMS

Materials — Recycling & Process Optimization II

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: John Howarter, Purdue University; Mingming Zhang, ArcelorMittal Global R&D; Elsa Olivetti, Massachusetts Institute of Technology; Hong Peng, University of Queensland

Wednesday PM March 17, 2021

Session Chair: Mingming Zhang, Arcelor Mittal Global R&D

2:00 PM

Ecodesign and Strategic Design of Alloys by Combinatorial Optimisation: *Franck Tancret*¹; Madeleine Bignon¹; Edern Menou²; Gérard Ramstein¹; Emmanuel Bertrand¹; Pedro Rivera-Diaz-Del-Castillo³; ¹University Of Nantes; ²Safran; ³Lancaster University

2:20 PM

Hydrometallurgical Recycling of Bauxite Residue: *Himanshu Tanvar*¹; Brajendra Mishra; ¹Worcester Polytechnic Institute

2:40 PM

Investigation of Ionic Liquids Isolated Iron for Ductile Iron Castings: Blake Stewart¹; Haley Doude¹; Morgan Abney²; Eric Fox²; Jennifer Edmunson²; Hongjoo Rhee¹; ¹Mississippi State University; ²National Aeronautics and Space Administration

3:00 PM

Uncertainty Analysis and Reduction for Environmental Impact Modeling of



Emerging Manufacturing Technologies: *Jiankan Liao*¹; Daniel Cooper¹; ¹University of Michigan

NUCLEAR MATERIALS

Thermal Property Characterization, Modeling, and Theory in Extreme Environments — Thermal Transport Theory & Mechanisms

Sponsored by: TMS Structural Materials Division, TMS: Nuclear Materials Committee

Program Organizers: Janelle Wharry, Purdue University; Mukesh Bachhav, Idaho National Laboratory; Marat Khafizov, Ohio State University; Eric Lass, University of Tennessee-Knoxville; Vikas Tomar, Purdue University; Tiankai Yao, Idaho National Laboratory; Cody Dennett, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Wednesday PM March 17, 2021

Session Chairs: Vikas Tomar, Purdue University; Mukesh Bachhav, Idaho National Laboratory; Karim Ahmed, Texas A&M University

2:00 PM Invited Thermal Transport in Irradiated ThO2: A Combined Experimental and Phonon Level Investigation: Anter El-Azab¹; *Walter Deskins*¹; Maniesha Singh¹; Sanjoy Mazumder¹; Kumagai Tomohisa¹; Jie Peng¹; Marat Khafizov²; Zilong Hua³; Lingfeng He³; David Hurley³; ¹Purdue University; ²Ohio State University; ³Idaho National Laboratory



2:30 PM Invited

Thermal Conductivity and Heat Transport Processes of Ion Irradiated and Laser Heated Solids: Patrick Hopkins¹; Thomas Pfeifer¹; Ethan Scott¹; John Gaskins¹; David Olson¹; Khalid Hattar²; Mark Goorsky³; ¹University of Virginia; ²Sandia National Labs; ³UCLA

3:00 PM

Thermal Gradient Effect on the Transport Properties of Helium and Intrinsic **Defects in Tungsten**: *Enrique Martinez Saez*¹; Nithin Mathew¹; Danny Perez¹; Dimitrios Maroudas²; Brian Wirth³; ¹Los Alamos National Laboratory; ²University of Massachusetts; ³University of Tennessee

3:20 PM Invited

Phonon Transport in ThO2 from Neutron Scattering and First-principles **Computation**: *Michael Manley*¹; Matthew Bryan¹; Chris Marianetti²; Lyuwen Fu²; Krzystof Gofryk³; ¹Oak Ridge National Laboratory; ²Columbia University; ³Idaho National Laboratory

3:50 PM Invited Theory of Non-equilibrium Thermal Transport at High Temperatures from Firstprinciples: *Keivan Esfarjani*¹; ¹University of Virginia

ADVANCED MATERIALS

2D Materials – Preparation, Properties & Applications – Modeling & **Simulations II**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces



Committee

Program Organizers: Nuggehalli Ravindra, New Jersey Institute of Technology; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Sufian Abedrabbo, Khalifa University; Amber Shrivastava, Indian Institute of Technology Bombay

March 18, 2021 Thursday AM

Session Chairs: Gerald Ferblantier, University of Strasbourg; Amber Shrivastava, Indian Institute of Technology

8:30 AM

Cesium Lead Bromides - Structural, Electronic & Optical Properties: Aneer Lamichhane¹; Nuggehalli Ravindra¹; ¹New Jersey Institute of Technology

8:50 AM

Thermoelectric Properties of 2-D B₄**C Nanosheets**: *Adway Gupta*¹; Arunima Singh¹; ¹Arizona State University

9:10 AM

Low Temperature Phonon Anharmonicity in Tungsten Diselenide: Qingan Cai¹; ¹University of California, Riverside

9:30 AM

Mechanism of Strain Transfer in Transition Metal Dichalcogenides for Phase **Change Transistors**: *Shoieb Ahmed Chowdhury*¹; Tara Peña¹; Stephen Wu¹; Hesam Askari¹; ¹University of Rochester



VEBSITE TMS



Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Thursday AM March 18, 2021

Session Chairs: Julie Tucker, Oregon State University ; Andrea Jokisaari, Idaho National Laboratory

8:30 AM

Compositionally Graded Bulk Specimen: A High-throughput Approach for Nuclear Alloy Development and Qualification: *Xiaoyuan Lou*¹; Jingfan Yang¹; Xiang Liu²; Miao Song³; Lingfeng He²; Yongfeng Zhang⁴; Daniel Schwen²; ¹Auburn University; ²Idaho National Lab; ³University of Michigan; ⁴University of Wisconsin-Madison

8:50 AM

A Superb Void Swelling Resistant Type 316L Stainless Steel Developed by Additive Manufacturing Enabled High Throughput Microalloying: *Miao Song*¹; Jingfan Yang²; Xiang Liu³; Xiaoyuan Lou²; Yongfeng Zhang⁴; Lingfeng He³; Daniel Schwen³; ¹University of Michigan; ²Auburn University; ³Idaho National Laboratory; ⁴University of Wiscousin

9:10 AM

Improving Irradiation Resistance of Alloys by Controlling Defect Diffusion: A Modeling Perspective: *Yongfeng Zhang*¹; Miao Song²; Xiang Liu³; Lingfeng He⁴; Daniel Schwen⁴; Xiaoyuan Lou⁵; ¹University of Wisconsin-Madison; ²University of Michigan ; ³Idaho National Laboratory ; ⁴Idaho National Laboratory; ⁵Auburn University

9:30 AM Invited

Role of Composition and Thermal Aging on Corrosion Behavior of Duplex Stainless Steels in Pressurized Water Reactors: *Julie Tucker*¹; Pratik Murkute¹; Kofi Oware Sarfo¹; Isak McGieson¹; Melissa Santala¹; Yongfeng Zhang²; Liney Arnadottir¹; Burkan Isgor¹; ¹Oregon State University; ²University of Wisconsin - Madison

10:00 AM

Development of Sintered High Strength and Thermal Conductivity Cu-Cr-Nb-Zr Alloy for Fusion Components: *Bin Cheng*¹; Ling Wang²; David Sprouster¹; Jason Trelewicz¹; Weicheng Zhong³; Ying Yang³; Steven Zinkle²; Lance Snead¹; ¹Stony Brook University; ²University of Tennessee, Knoxville; ³Oak Ridge National Laboratory

10:20 AM

Evaluation of Creep Deformation of Ferritic/Martensitic (FM) Grade 91 Steel Fabricated Using Wire Arc Additive Manufacturing (WAAM): *Mahmoud Hawary*¹; K. Murty¹; ¹North Carolina State University

Additive Manufacturing of Functional, Energy, and Magnetic Materials —

Additive Manufacturing of NiTi

Sponsored by: TMS Functional Materials Division, TMS: Additive Manufacturing Committee, TMS: Magnetic Materials Committee

Program Organizers: Markus Chmielus, University of Pittsburgh; Sneha Prabha Narra, Worcester Polytechnic Institute; Mohammad Elahinia, University of Toledo; Reginald Hamilton, Pennsylvania State University; Iver Anderson, Iowa State University Ames Laboratory

Thursday AM March 18, 2021

8:30 AM

Composition Control in Laser Powder Bed Fusion Additive Manufacturing Through Differential Evaporation: *Meelad Ranaiefar*¹; Ibrahim Karaman¹; Alaa Elwany¹; Raymundo Arroyave¹; ¹Texas A&M University

8:50 AM

Toward Understanding the Effect of Selective Laser Re-melting on the Mechanical Properties of the SLM Fabricated Nitinol: *Parisa Bayati*¹; Keyvan Safaei¹; Mohammadreza Nematollahi¹; Ahmadreza Jahadakbar²; Mohammad Mahtabi³; Mohammad Elahinia¹; ¹The University of Toledo; ²Thermomorph LLC; ³The University of Tennessee at Chattanooga

9:10 AM

Selective Laser Melting of Defect-free NiTiSMAParts Using a Process Optimization Framework: *Lei Xue*¹; Chen Zhang¹; Kadri Atli¹; Bing Zhang¹; Alaa Elwany¹; Raymundo Arroyave¹; Ibrahim Karaman¹; ¹TAMU



MOBILE-FRIENDL

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Beyond the Beam II — Deformation Based Processing

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Paul Prichard, Kennametal Inc.; James Paramore, US Army Research Laboratory; Peeyush Nandwana, Oak Ridge National Laboratory; Nihan Tuncer, Desktop Metal

Thursday AM March 18, 2021

Session Chair: James Paramore, Texas A&M University

8:30 AM

In Situ Monitoring of Additive Friction Stir Deposition: An Overview: Hang Yu¹; ¹Virginia Polytechnic Institute and State University

8:50 AM

Texture Development and Influence in Solid-state Additive Manufacturing: *Robert Griffiths*¹; Mackenzie Perry¹; David Garcia¹; Hang Yu¹; ¹Virginia Polytechnic Institute

9:10 AM

Complex Material Deformation and Flow Phenomena during Additive Friction Stir Deposition of Dissimilar Aluminum Alloys: *Mackenzie Perry*¹; Hunter Rauch¹; Robert Griffiths¹; Jennifer Sietins²; Yunhui Zhu¹; David Garcia¹; Hang Yu¹; ¹Virginia

Tech; ²CCDC Army Research Laboratory

TMS WEBSITE **ADDITIVE TECHNOLOGIES**

9:30 AM

Friction Stir Additive Manufacturing of Al 6061-T6: Modeling and Experimental **Analysis**: Nitin Rohatgi¹; *Yung Shin*¹; ¹Purdue University

9:50 AM Cold Spray Processing of Soft Metals and Hard Tool Steels: Yu Zou¹; ¹University of Toronto

10:10 AM

Heat Treatment of Recycled Battlefield Stainless-Steel Scrap for Cold Spray Applications: Christopher Massar¹; Kyle Tsaknopoulos¹; Bryer Sousa¹; Jack Grubbs¹; Danielle Cote¹; ¹Worcester Polytechnic Institute

10:30 AM

Understanding the Effects of Repeated Environmental Exposure on Powder **Properties for Additive Manufacturing Applications**: *Jack Grubbs*¹; Aaron Birt²; Aaron Nardi³; Danielle Cote¹; ¹Worcester Polytechnic Institute; ²Solvus Global; ³Army Research Lab

10:50 AM

Aluminum Alloy Powders for Solid State Additive Manufacturing Processing: *Kyle Tsaknopoulos*¹; Jack Grubbs¹; Danielle Cote¹; ¹Worcester Polytechnic Institute

11:10 AM

Linear Friction Welding: a Solid-state Joining Process for the Manufacturing of **Aerospace Titanium Parts**: *Nicolas Piolle*¹; ¹ACB

CONTENTS

TABLE

Q

MOBILE-FRIEND

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Aluminium Alloys

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

Thursday AM March 18, 2021

Session Chairs: Whitney Poling, General Motors; Andrew Wessman, The University of Arizona

8:30 AM Invited **Connecting Microstructure Evolution to Mechanical Behavior of an Al-Mn-Sc** Alloy Designed for Selective Laser Melting: Fan Zhang¹; Qingbo Jia²; Xinhua Wu²; ¹National Institute of Standards and Technology; ²Monash University

9:00 AM

Characterization and Simulation of Eta and Eta-prime Precipitates Evolution in Laser Heat Treated Cold Spray of AA7050: Ning Zhu¹; Luke Brewer¹; ¹University of Alabama



9:20 AM

Possibilities for Replacing Scandium in High Strength Al-Mg Alloys for 3D Printing by Transition Metal Alloying: Viktor Mann¹; Roman Vakhromov²; Dmitriy Ryabov²; Vladimir Korolev²; Daria Daubarayte²; Maria Grol²; Alexander Seferyan²; Kirill Nyaza²; ¹RUSAL Management; ²Light Materials and Technologies Institute

9:40 AM

Solidification Structure Characterization of an AlCuMnZr Alloy with respect to geometric features and Multiple Parameters: Kevin Sisco¹; Sumit Bahl²; Matthew Chisholm²; Richard Michi²; Jonathan Poplawsky²; Amit Shyam²; Ryan Dehoff²; Alex Plotkowski²; Suresh Babu¹; ¹University of Tennessee Knoxville; ²Oak Ridge National Lab

10:00 AM

Effects of Thermal Processing on the Microstructure and Mechanical Properties of Additively Manufactured AlSi10Mg Parts: John Fite¹; Suhas Prameela²; John Slotwinski¹; Timothy Weihs²; ¹Jhu Applied Physics Lab; ²Johns Hopkins University

10:20 AM

Evolution of Microstructure and Dispersoids in Al-Mg 5xxx Alloys Under Wire + Arc Additive Manufacturing and Permanent Mold Casting: Kun Liu¹; Ahmed Algendy¹; Jianglong Gu²; X. Grant Chen¹; ¹University of Quebec at Chicoutimi; ²Yanshan University

10:40 AM

Effect of Laser Glazing on Powder-Processed Icosahedral-Phase-Strengthened Aluminum Alloys: From Single Track to Overlapping Tracks: *Mingxuan Li*¹; Hannah Leonard¹; Sarshad Rommel¹; Cain Hung¹; Thomas Watson²; Tod Policandriotes³; Rainer Hebert¹; Mark Aindow¹; ¹University of Connecticut; ²Pratt & Whitney; ³Collins



THURSDAY AM

CONTENTS

TABLE

Q

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation — Session VII**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara

; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

March 18, 2021 **Thursday AM**

8:30 AM

Materials Processing in a Synchrotron Beam: Klaus-Dieter Liss¹; ¹Guangdong Technion - Israel Institute of Technology (GTIIT)

8:50 AM

On the Coupled Effects of Hydrogen Diffusion and Hydride Precipitation in **Zirconium Alloys**: *Alireza Tondro*¹; Hamidreza Abdolvand¹; ¹Western University



9:10 AM

Crystal Plasticity-based Modelling of Taylor Impact Test of Single Crystal Tantalum: Zhangxi Feng¹; Miroslav Zecevic²; Ricardo Lebensohn²; Marko Knezevic¹; ¹University of New Hampshire; ²Los Alamos National Laboratory

9:30 AM Slip-twin Transfer Across Phase Boundaries: An In-situ Investigation of a Ti-Al-V-Fe (a+B) Alloy : Shaolou Wei¹; Gaoming Zhu¹; Cem Tasan¹; ¹Massachusetts Institute of Technology

9:50 AM

Variability in Mechanical Properties Related to Porosity in LMD Waspaloy: Azdine Nait-Ali¹; Romain Bordas¹; Roland Fortunier¹; Patrick Villechaise¹; Lucie Rat²; Sebastien Rix²; Samuel Hemery¹; Jonathan Cormier¹; ¹Isae Ensma; ²Safran Aircraft Engines

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Coating **Technologies and Surface Structuring for Tools II**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra,



THURSDAY AM

NTENTS

Π

9

New Jersey Institute of Technology; Vikas Tomar, Purdue University

Thursday AM March 18, 2021

Session Chairs: Heinz Palkowski, IMET; Ravindra Nuggehalli, New Jersey Institute of Technology

8:30 AM Invited

Nanoengineered Coating; Lotus Effect, Morphology, Contact Angles and Wettability: Narsingh Singh¹; Lisa Kelly¹; Narasimha Prasad¹; Brett Setera¹; Stacey Sova¹; David Sachs¹; Bradley Arnold¹; Fow-Sen Choa¹; Christopher Cooper¹; ¹University of Maryland, Baltimore County

9:00 AM

High-quality Diamond Films on Q-carbon Coated Austenitic Stainless Steels **304 and 316**: *Pratik Joshi*¹; Siddharth Gupta²; Ariful Haque²; Jagdish Narayan²; ¹NC State University; ²Intel Corporation

9:20 AM

Ni-Zn-Al2O3 Cermet Nanocomposite Coatings by High-pressure Cold Spraying: Jagannadh Sripada¹; Gobinda Saha¹; ¹University of New Brunswick

9:40 AM Invited Manipulating Polyolefin Performance by Control of Morphology through **Processing**: *Michael Jaffe*¹; ¹New Jersey Innovation institute

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Multifunctional

TMS

Biomaterials, Innovative Approaches to New Concepts and Applications II

WEBSITE

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

Thursday AM March 18, 2021

Session Chairs: Adele Carrado, Université de Strasbourg IPCMS; Heinz Palkowski, IMET

8:30 AM Keynote Diamond-like Coatings: A Flexible Platform for Multifunctional Antibacterial **Coatings for Health**: Linda Bonilla¹; Pascale Chevallier¹; *Diego Mantovani*¹; ¹Laval University

9:10 AM Invited Grafting of Bioactive Polymers with Various Architectures for Preparing Antibacterial and Biocompatible Surfaces: Céline Falentin-Daudre¹; Véronique Migonney¹; ¹LBPS-CSPBAT

9:40 AM

On the Controlled Antibacterial Activity of a Silver Oxide Doped Diamond-like Carbon Nanocoating With a Semi-permeable Polymeric Top Layer for Longterm Stability: Linda Bonilla-Gameros¹; Pascale Chevallier¹; Diego Mantovani¹;

¹Laboratory for Biomaterials and Bioengineering, Laval University

10:00 AM Keynote

Biomimetic Calcium-deficient Hydroxyapatite Coating on Activated Carbon Fiber Cloth: A Dual Drug Delivery System: Sylvie Bonnamy¹; ¹CNRS

10:40 AM

DesignofTi-copolymerSandwichesforBiomedicalImplanttoImproveFormability: Flavien Mouillard; Patrick Masson¹; Genevieve Pourroy¹; Adele Carrado¹; ¹IPCMS -CNRS

11:00 AM

Design of Innovative Hybrid Structures Using Grafting of Architecture-controlled Polymers for Biomedical Applications: Caroline Pereira¹; Jean-Sébastien Baumann¹; Patrick Masson²; Geneviève Pourroy²; Heinz Palkowsky³; Adele Carradò²; Véronique Migonney¹; Céline Falentin-Daudré¹; ¹LBPS/CSPBAT, UMR CNRS 7244, Institut Galilée, Université Sorbonne Paris Nord; ²Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), UMR 7504 CNRS, Université de Strasbourg; ³Clausthal University of Technology (TUC), IMET Institute of Metallurgy

11:20 AM

Forming Limits and Shaping of Ti-PMMA-Ti Sandwiches for Biomedical Applications: Gargi Nayak¹; Heinz Palkowski¹; ¹TU Clausthal

ENERGY & ENVIRONMENT

Advanced Magnetic Materials for Energy and Power Conversion Applications - Developments in Emerging Permanent Magnets



Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

Thursday AM March 18, 2021

Session Chairs: Yongmei Jin, Michigan Technological University; Zachary Morgan, Oak Ridge National Laboratory

8:30 AM

Atomic Cooperation in Enhancing Magnetism: (Fe, Cu)-doped CeCo5: Durga *Paudyal*¹; Renu Choudhary¹; ¹Ames Laboratory

8:50 AM Computational Modeling of Fracture in Sm-Co Magnet: *Ikenna Nlebedim*¹; Xubo Liu¹; Baozhi Cui¹; Jun Cui¹; ¹Ames Laboratory

9:10 AM

Effects of Lattice Distortions on Magnetic Properties of Fe16N2: First-principles Study: Yusuke Asari¹; Tomohiro Tabata¹; Shinya Tamura¹; Matachiro Komuro¹; Shohei Terada¹; ¹Hitachi, Ltd.

9:30 AM

Heterogeneous Sm-Co Sintered Magnets with Enhanced Mechanical Properties:



*Baozhi Cui*¹; Xubo Liu¹; Gaoyuan Ouyang¹; Cajetan Nlebedim¹; Jun Cui¹; ¹Ames Laboratory

9:50 AM Invited

MnBi Thin Film Micromagnets with Tunable Anisotropy for High Temperature Applications: M. Villanueva¹; E. H. Sánchez²; P. Pedraz¹; P. Olleros¹; P. Perna¹; P. S. Normile²; C. Navío¹; J. Camarero¹; *Jose De Toro*²; A. Bollero¹; ¹IMDEA Nanoscience, Madrid, Spain; ²IRICA & Applied Physics Dept, University of Castilla-La Mancha, Spain

10:20 AM

Role of Fe in Stabilizing Ce(Co, Fe, Cu), and Enhancing Its Magnetic Properties: *Matthew Kramer*¹; Oleana Palasyuk¹; Tae-Hoon Kim¹; Lin Zhou¹; Sergey Budko¹; Paul Canfield¹; Andriy Palasyuk¹; ¹Ames Laboratory

10:40 AM

Evaluation of Medium-entropy FexCoyNiz Alloys as Precursors for FeCoNi**based High Entropy Magnetic Alloys**: Alex Paul¹; *Tanjore Jayaraman*¹; ¹University of Michigan-Dearborn

11:00 AM

Substitutional and Interstitial Doping in 1-5 and Its Derivative Structures for the **Development of Hard Magnetic Properties: A First Principles Study**: *Huseyin Ucar*¹; Durga Paudyal²; ¹California Polytechnic University, Pomona; ²Ames Laboratory

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Energy Storage with Emphasis on Batteries II



Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Thursday AM March 18, 2021

Session Chairs: Eric Detsi, University of Pennsylvania; Scott Roberts, Sandia National Laboratory

8:30 AM

MesoscaleMechanics:SimulatingtheRoleofStressonElectrodeElectrochemical Performance: Scott Roberts¹; Mark Ferraro¹; Jeffrey Horner¹; Julia Meyer²; Benjamin Ng¹; ¹Sandia National Laboratories; ²Purdue University

9:00 AM

Metal-sulfur nanocomposite for developing high-loading electrochemical cathode: Sheng-Heng Chung¹; *Cun-Sheng Cheng*¹; ¹National Cheng Kung University

9:20 AM

Molecular-level Characterization of the Electrode-electrolyte Interfaces in Li Batteries: Lauren Marbella¹; ¹Columbia University

9:50 AM

New Insights Linking Material Properties and Performance of the Lithium SEI:



*Betar Gallant*¹; ¹MIT

10:20 AM

Simulations of Phase Transformation in Complex Graphite Electrode Microstructures: *Affan Malik*¹; Kent Snyder²; Minghong Liu²; Hui-Chia Yu¹; ¹Michigan State University; ²Ford Auto Company

MATERIALS DESIGN

Advances in Titanium Technology — Powder Metallurgy and Additive Manufacturing of Ti and Ti Alloys

Sponsored by: TMS Structural Materials Division, TMS: Titanium Committee

Program Organizers: Don Li, Howmet Engineered Products; Yufeng Zheng, University of Nevada-Reno ; Peeyush Nandwana, Oak Ridge National Laboratory; Matthew Dunstan, US Army Research Laboratory

Thursday AM March 18, 2021

Session Chair: Matthew Dunstan, U.S. Army Research Laboratory

8:30 AM

Development of Cold Spray Additive Technology for Manufacturing Titanium Mill Products: *Stefan Gulizia*¹; Leon Prentice¹; Peter King¹; Saden Zahiri¹; Alejandro Vargas Uscategui¹; Christian Doblin¹; ¹CSIRO Manufacturing

8:50 AM Investigation to Hole Surface Microstructure Evolution in Drilling of

TMS

Aerospace Alloys: Ti-5553

9:10 AM

Process Design for Laser Hot Wire Additive Manufacturing of Ti-6Al-4V: Brandon Abranovic¹; Elizabeth Chang-Davidson¹; Jack Beuth¹; ¹Carnegie Mellon University

9:30 AM

Opportunities to Develop Superior Titanium Alloys by Laser Powder Bed Fusion: *Marco Simonelli*¹; Graham McCartney¹; Zou Zhiyi¹; Nesma Aboulkhair¹; Yau Yau Tse¹; Adam Clare¹; Richard Hague¹; ¹University of Nottingham

9:50 AM

Towards an ICME Framework of Designing Post-process for Additively ManufacturedTi-6Al-4V: ShengyenLi¹; Kirby Matthew¹; James Sobotka¹; ¹Southwest **Research Institute**

MATERIALS DESIGN

AI/Data informatics: Tools for Accelerated Design of High-temperature Alloys - Al Design and Thermodynamics

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Michael Titus, Purdue University; Pinar Acar, Virginia Tech; Andrew Detor, GE Research; James Saal, Citrine Informatics; Dongwon Shin, Oak Ridge National Laboratory



Thursday AM March 18, 2021

Session Chairs: Pinar Acar, Virginia Tech; Michael Titus, Purdue University

8:30 AM Invited Knowledge-driven Platform for Federated Multimodal Big Data Storage & **Analytics**: *Kareem Aggour*¹; Vipul Gupta¹; Andy Detor¹; Scott Oppenheimer¹; Joe Vinciquerra¹; ¹GE Research

9:00 AM

Exploring the Compositional Space of High Entropy Alloys via Sequential Learning: Juan Verduzco¹; Zachary McClure¹; David Farache¹; Saaketh Desai¹; Alejandro Strachan¹; ¹Purdue University

9:20 AM

Uncertainty Reduction for Calculated Phase Equilibria: *Richard Otis*¹; Brandon Bocklund²; Zi-Kui Liu²; ¹Jet Propulsion Laboratory; ²Pennsylvania State University

9:40 AM

Predicting Vibrational Entropy of FCC Solids Uniquely from Bond Chemistry Using Machine Learning: Anus Manzoor¹; Dilpuneet Aidhy¹; ¹University of Wyoming

LIGHT METALS

Aluminum Reduction Technology — Environment (Material and Equipment)



Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Nadia Ahli, Emirates Global Aluminium; Nancy Holt, Hydro Aluminium AS

Thursday AM March 18, 2021

Session Chair: Shane Polle, EGA

8:30 AM

Low and High Voltage PFC Slope Coefficient Monitoring during Pot Start-up: Christine Dubois¹; *Luis Espinoza-Nava*¹; ¹Alcoa

8:50 AM

Latest Developments in GTC Design to Reduce Fluoride Emissions: *Philippe Martineau*¹; Youssef Joumani¹; Bassam Hureiki¹; Jérémy Neveu¹; Fabienne Virieux¹; ¹Fives

9:10 AM

Process and Environmental Aspects of Applying Unshaped Carbon Materials for Cell Lining Purposes: *Alexander Proshkin*¹; Vitaly Pingin¹; Viktor Mann¹; Aleksey Zherdev¹; Andrey Sbitnev¹; Yury Shtefanyuk¹; ¹RUSAL

9:30 AM

Characterisation of Powders-precondition for Plant Engineering: Peter Hilgraf¹; Arne Hilck²; *Jan Paepcke*²; ¹HAW, Hamburg, University of Applied Science; ²Claudius Peters Projects GmbH



MOBILE-FRIEND

9:50 AM

Gas Treatment in the GE Pot Integrated ABART Modules (PIA): Anders Sorhuus¹; Håvard Olsen¹; Eivind Holmefjord¹; Roger Theodorsen¹; Mikkel Sørum¹; ¹GE Power

10:10 AM

New Phase in Upgrade of Søderberg Technology at RUSAL's Smelters: *Viktor Buzunov*¹; Viktor Mann²; Vitaliy Pingin¹; Aleksey Zherdev¹; Maksim Kazantsev¹; Andrey Pinaev¹; Yuriy Bogdanov¹; ¹Rusal Etc; ²UC RUSAL

10:30 AM Question and Answer Period

BIOMATERIALS

Biological Materials Science — Biological Materials Science III

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Biomaterials Committee

Program Organizers: David Restrepo, University of Texas at San Antonio; Steven Naleway, University of Utah; Jing Du, Pennsylvania State University; Ning Zhang, University of Alabama

Thursday AM March 18, 2021

Session Chairs: Santiago Orrego, Temple University; Alexander Ossa, Universidad EAFIT

8:30 AM Invited Microstructural Variations in Mammalian Enamel: An Exploration of Decussation from the Micro- to the Macro-scale: Cameron Renteria¹; Juliana Fernández-Arteaga²; Alexander Ossa²; *Dwayne Arola*¹; ¹University of Washington; ²Universidad

EAFIT

9:00 AM

On the Structure and Mechanical Properties of Aprismatic Enamel in Crocodilian **Teeth**: Jack Grimm¹; Cameron Renteria¹; Savannah Camacho¹; Xitlalit Sanchez-Martinez¹; Dwayne Arola¹; ¹University of Washington

9:20 AM

Tough Enlightenments From the Prayer Bead: Fracture-tolerant Endocarp of *Elaeocarpus Ganitrus* Seed (Rudraksha): *Ashish Ghimire*¹; Po-Yu Chen¹; ¹National Tsing Hua University

9:40 AM Invited Bioinspired Graphene Nanocomposites with Exceptionally High Mechanical **Performance**: *Xiaodong Li*¹; ¹University of Virginia

10:10 AM Invited Tapes: An Overlooked Biological Material Archetype: Hannes Schniepp¹; ¹College of William & Mary

10:40 AM Invited Mechanical Properties of Tough, Mechanochemically Active Hydrogels and Hydrogel-based Composites: Jamie Kruzic¹; Yuwan Huang¹; Bhakthi Jayathilaka¹; Shariful Islam¹; Meredith Silberstein²; Kristopher Kilian¹; ¹University of New South Wales; ²Cornell University



Bulk Metallic Glasses XVIII — Structures and Mechanical Properties

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Thursday AM March 18, 2021

Session Chairs: Jamie Kruzic, University of New South Wales; Xie Xie, FCA US LLC

8:30 AM Invited

Microstructure - Fracture Toughness Relationships in Bulk Metallic Glasses: Jamie Kruzic¹; Bosong Li¹; Bernd Gludovatz¹; Anna Ceguerra²; Keita Nomoto¹; Simon Ringer²; Shenghui Xie³; Sergio Scudino⁴; ¹University of New South Wales; ²The University of Sydney; ³Shenzhen University; ⁴IFW Dresden

8:55 AM Invited StructuralHeterogeneitiesDictateStrengthandFractureToughnessinaZr-based Metallic Glass: Bernd Gludovatz¹; Lisa Krämer²; Bosong Li¹; Anton Hohenwarter³; Jamie Kruzic¹; ¹UNSW Sydney; ²ESI-Leoben; ³Montanuniversität Leoben

9:20 AM Invited Mechanical Behavior and Phase Stability of Ductile Metallic Glass Nanoparticles: Wendy Gu¹; Mehrdad Kiani¹; Abhinav Parakh¹; ¹Stanford University



8:30 AM Simulation-based Analysis for Optimization of Casting Process in AA7075: Siamak Rafiezadeh¹; *Philip Pucher*¹; Steffen Neubert¹; Waldemar Ivanov¹; ¹AMAG

9:45 AM Invited

Microscopic Description of Plasticity, Relaxation and Rejuvenation Using Anelastic Relaxation Spectra: Michael Atzmon¹; Tianjiao Lei²; Luis Rangel DaCosta³; ¹University of Michigan; ²University of California, Irvine; ³University of California, Berkeley

10:10 AM

Competing Effects of Topology and Chemical Bonding on Mechanical Properties of Metallic Glasses: Vrishank Jambur¹; Chaiyapat Tangpatjaroen¹; Jianqi Xi¹; Meng Gao¹; John Perepezko¹; Izabela Szlufarska¹; ¹University of Wisconsin - Madison

LIGHT METALS

Cast Shop Technology — DC Casting

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizer: Samuel Wagstaff, Oculatus

Thursday AM March 18, 2021

Session Chairs: Philippe Jarry, Constellium; Samuel Wagstaff, Oculatus

THURSDAY AM



MOBILE-FRIEND

8:50 AM

Characterization of Ingots Cast with the APEX™ Casting System: Craig Cordill¹; Gerhard Castro¹; Bin Zhang¹; ¹Wagstaff

9:10 AM

Effect of Ultrasonic Melt Treatment on the Sump Profile and Microstructure of a Direct-chill Cast AA6008 Aluminum Alloy: *Tungky Subroto*¹; Gerard Serge Bruno Lebon¹; Dmitry Eskin¹; Ivan Skalicky²; Dan Roberts²; Iakovos Tzanakis³; Koulis Pericleous⁴; ¹Brunel University London; ²Constellium UTC; ³Oxford Brookes University; ⁴University of Greenwich

9:30 AM

The Influence of the Casting Speed in Horizontal Continuous Casting of Aluminium Alloy EN AW 6082: Akin Obali¹; Kerem Dilek¹; Mertol Gokelma²; Seracettin Akdi³; Deniz Kavrar Ürk¹; ¹Sistem Teknik Industrial Furnaces Ltd.; ²Izmir Institute of Technology; ³Akdi Engineering and Consultancy

9:50 AM

The Impact of Casting Conditions on Edge Cracking of AA5182 Ingots during Hot **Rolling**: *Samuel Wagstaff*¹; ¹Oculatus

10:10 AM

Reducing Gas Shrinkage Porosity in AlMg Alloy Slabs: Igor Kostin¹; Aleksandr Sidorov¹;AlekseyStartsev¹;AndreyKrechetov¹;AleksandrKrokhin¹;SergeyBelyaev²; ¹UC RUSAL; ²SFU

10:30 AM

Molecular Dynamics Simulations of the Evolution of Residual Stresses during **Rapid Solidification of Aluminium**: *Michail Papanikolaou*¹; Konstantinos Salonitis¹; Mark Jolly¹; ¹Cranfield University

10:50 AM Question and Answer/Panel Discussion

VEBSITE TMS



NUCLEAR MATERIALS

Ceramic Materials for Nuclear Energy Research and Applications — Radiation Effects and Mass Transport

Sponsored by: TMS Extraction and Processing Division, TMS Structural Materials Division, TMS Light Metals Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Committee, TMS: Nuclear Materials Committee

Program Organizers: Xian-Ming Bai, Virginia Polytechnic Institute and State University; Yongfeng Zhang, University of Wisconsin-Madison; Larry Aagesen, Idaho National Laboratory; Vincenzo Rondinella, Jrc-Ec

Thursday AM March 18, 2021

Session Chairs: Simon Pimblott, Idaho National Laboratory; Walter Luscher, Pacific Northwest National Laboratory

8:30 AM Invited Irradiation Effects on Zirconium Alloy Oxides and Their Impacts on In-reactor Corrosion Rates: *Adrien Couet*¹; Zefeng Yu¹; Taeho Kim¹; Hongliang Zhang¹; Mukesh Bachhav²; Lingfeng He²; ¹University of Wisconsin-Madison; ²Idaho National Laboratory

9:00 AM Effect of UV and Gamma Irradiation on the Hydrothermal Corrosion of Ionirradiated SiC: *Arunkumar Seshadri*¹; Koroush Shirvan¹; Taeho Kim²; Adrien Couet²; ¹Massachusetts Institute of Technology; ²University of Wisconsin-Madison

9:20 AM Invited In-situ Measurement of Tritium Release from Lithium Aluminate Under Neutron Irradiation: *Walter Luscher*¹; David Senor¹; Gary Hoggard²; ¹Pacific Northwest National Laboratory; ²Idaho National Laboratory

9:50 AM

Influence of Dose Rate and Temperature on Mass Transport in Hematite: Kayla Yano¹; Sandra Taylor¹; Tiffany Kaspar¹; Danny Edwards¹; Daniel Schreiber¹; ¹Pacific Northwest National Laboratory

10:10 AM

Radiation Tolerance of Nanoporous Gadolinium Titanate: Nathan Madden¹; Matthew Janish²; James Valdez²; Blas Uberuaga²; Jessica Krogstad¹; ¹University of Illinois at Urbana-Champaign; ²Los Alamos National Laboratory

10:30 AM

Radiolytic Damage and Hydrogen Generation at Carbide – Water Interfaces: Simon Pimblott¹; Jay LaVerne²; ¹Idaho National Laboratory; ²University of Notre Dame

10:50 AM

Molecular Dynamics Investigations of AlN-based Piezoelectric Ceramics under Irradiation: *Michael Kempner*¹; Jesse Sestito¹; Eva Zarkadoula²; Yan Wang¹; ¹Georgia Institute of Technology; ²Oak Ridge National Laboratory

11:10 AM

Irradiation Damage in High-entropy Carbide Ceramics: Fei Wang¹; Xueliang Yan¹; Tianyao Wang²; Yaqiao Wu³; Lin Shao²; Michael Nastasi²; Yongfeng Lu¹; *Bai Cui*¹;

¹University of Nebraska-Lincoln; ²Texas A&M University; ³Boise State University

CHARACTERIZATION



Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Richard Sandberg, Brigham Young University; Ross Harder, Argonne National Laboratory; Xianghui Xiao, Brookhaven National Laboratory; Brian Abbey, La Trobe University; Saryu Fensin, Los Alamos National Laboratory; Ana Diaz, Paul Scherrer Institut; Mathew Cherukara, Argonne National Laboratory

Thursday AM March 18, 2021

Session Chair: Xianghui Xiao, Brookhaven National Laboratory

8:30 AM Invited In Situ and Operando 3D Nano-imaging for Materials Science at the ESRF: Julie Villanova¹; Richi Kumar¹; Victor Vanpeene¹; Jaime Segura-Ruiz¹; Remi Tucoulou¹; Pierre Lhuissier²; Luc Salvo²; ¹ESRF; ²SIMAP/UGA

9:00 AM Evaluation of TATB Crystal Morphology for Predicting Sensitivity Using X-ray Computed Tomography: *Lindsey Kuettner*¹; Brian Patterson¹; John Yeager¹; Larry Hill¹; ¹Los Alamos National Laboratory **MOBILE-FRIEND**

9:20 AM

Megahertz X-ray Microscopy for Imaging High-speed Phenomena in Opaque Materials: *Valerio Bellucci*¹; Tokushi Sato¹; Pablo Villanueva Perez²; Jozef Ulicny³; Wataru Yashiro⁴; Henry Chapman⁵; Adrian Mancuso¹; Patrik Vagovic⁵; ¹European XFEL GmbH; ²Lund University; ³Pavol Jozef Šafárik University; ⁴Tohoku University; ⁵Center for Free-Electron Laser Science

9:40 AM

Microstructural Characterization and Mechanical Behavior of a Meteorite Using Correlative Microscopy: *Tai-Jan Huang*¹; Sridhar Niverty¹; Arun Sundar¹; Md Fazle Rabbi²; Laurence Garvie²; Aditi Chattopadhyay²; Desireé Cotto-Figueroa³; Nikhilesh Chawla¹; ¹Purdue University; ²Arizona State University; ³University of Puerto Rico at Humacao

10:00 AM Invited

Imaging Materials on the Run: Shedding Light on Fast Structural Processes Using Time-resolved Synchrotron X-ray Tomographic Microscopy: *Christian Schlepütz*¹; Federica Marone¹; Anne Bonnin¹; Marco Stampanoni¹; ¹Paul Scherrer Institute

10:30 AM

Quantitative Data Analysis of Dynamic Tomography Data with Motion Artifacts: *Xianghui Xiao*¹; Yang Yang¹; Zhenrui Xu²; James Steiner²; Yijin Liu³; Feng Lin²; ¹Brookhaven National Laboratory; ²Virginia Tech; ³SLAC National Accelerator Laboratory

10:50 AM Invited

High Speed, High Resolution, High Temperature 3D Imaging of Spacecraft Materials during Atmospheric Entry Conditions: *Dilworth Parkinson*¹; Harold Barnard¹; Alastair MacDowell¹; Sam Schickler¹; Shawn Shacterman¹; Talia Benioff-White¹; Kara Levy¹; Francesco Panerai²; Collin Foster²; Benjamin Ringel²; Christian Schlepuetz³; ¹Lawrence Berkeley National Laboratory; ²University of Illinois,

TMS

Urbana-Champaign; ³Paul Scherrer Institute

MOBILE-FRIEND

TABLE

Q

ONTENTS

11:20 AM

Study of Structure of Beam-sensitive Supported Nanoparticle Catalysts by Lowdose High Resolution Phase Contrast Imaging: Cheng-Han Li¹; Joerg Jinschek¹; ¹The Ohio State University

11:40 AM

Indexing Grains: A Comparison between Three-dimensional Synchrotron X-ray **Diffraction and Electron Backscatter Diffraction Techniques**: Karim Louca¹; Hamidreza Abdolvand¹; ¹Western University

ADDITIVE TECHNOLOGIES

Computational Techniques for Multi-Scale Modeling in Advanced Manufacturing — Multiscale Solidification Models

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Extraction and Processing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, University of Alabama; Mei Li, Ford Motor Company; Alexandra Anderson, Gopher Resource; Srujan Rokkam, Advanced Cooling Technologies Inc

Thursday AM March 18, 2021

Session Chair: Anthony Rollett, Carnegie Mellon



8:30 AM

ComputationalMulti-ScaleModelingofSegregationandMicrostructureEvolution during the Solidification of A356 Ingots Processed via a 2-Zone Induction Melting **Furnace**: Aqi Dong¹; *Laurentiu Nastac*¹; ¹University of Alabama

8:55 AM

Microstructural Evolution and Defect Formation During Pulsed and Continuous Selective Laser Melting: Ian Mccue¹; Steven Storck¹; James Mastandrea¹; Morgana Trexler¹; ¹Johns Hopkins Applied Physics Laboratory

9:20 AM

Computational Modeling of Nanoparticles Dispersion in Hybrid Process of Ink Jetting and Laser Powder Bed Fusion: *Milad Ghayoor*¹; Bryce Cox¹; Joshua Gess¹; Somayeh Pasebani¹; ¹Oregon State University

9:45 AM

Multi-scale, Multi-physics Modeling of Additive Manufacturing: Challenges and **Potential Solutions**: *Dayalan Gunasegaram*¹; Anthony Murphy¹; ¹CSIRO

10:10 AM

Multiphysics Simulation of Microstructure Evolution in Selective Laser Melting of AlSi10Mg: Dehao Liu¹; Yan Wang¹; ¹Georgia Institute of Technology

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics — Data Methods, Tools and High Throughput



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

March 18, 2021 **Thursday AM**

Session Chairs: Rodrigo Freitas, Stanford University; Dehao Liu, Georgia Institute of Technology; Arunima Singh, Arizona State University; Raymundo Arroyave, Texas A&M University

8:30 AM Invited Data-driven Discovery of Materials for Photocatalytic Energy Conversion: Arunima *Singh*¹; ¹Arizona State University

9:00 AM

High-throughput Density-functional Theory Methods for Discovery of Actinide Materials: *Matthew Christian*¹; Erin Johnson²; Theodore Besmann¹; ¹University of South Carolina; ²Dalhousie University

9:20 AM Invited The High Entropy Alloy Space is Not as Big as We Think It is: Raymundo Arroyave¹; Tanner Kirk¹; ¹Texas A&M University

MOBILE-FRIEND

9:50 AM Invited **Uncovering Atomistic Mechanisms of Crystallization Using Machine Learning:** *Rodrigo Freitas*¹; Evan Reed²; ¹Massachusetts Institute of Technology; ²Stanford University

10:20 AM Invited A Data-driven Approach to Long-Time Molecular Dynamics: Danny Perez¹; Nithin Mathew¹; Enrique Martinez¹; ¹Los Alamos National Laboratory

10:50 AM Invited Dendritic Growth Prediction in Metal Additive Manufacturing with Physicsconstrained Neural Networks: Dehao Liu¹; Yan Wang¹; ¹Georgia Institute of Technology

CORROSION

Environmental Degradation of Additively Manufactured Alloys — AM Materials and Aqueous Corrosion - Part II: Stainless Steel, Inconel 718 and Coatings

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Additive Manufacturing Committee

Program Organizers: Kinga Unocic, Oak Ridge National Laboratory; Jenifer Locke, Ohio State University; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Xiaoyuan Lou, Auburn University; Brendy Rincon Troconis, University of Texas at San Antonio; Luke Brewer, University of Alabama

Thursday AM March 18, 2021



Session Chairs: Brendy Rincon Troconis, University of Texas at San Antonio; Luke Brewer, University of Alabama

8:30 AM

Localized Corrosion of Additively Manufactured Stainless Steels: Michael Melia¹; Jesse Duran¹; Rebecca Marshall²; Ryan Katona²; Rebecca Schaller¹; Jeffrey Rodelas¹; Michael Heiden¹; Bradley Jared¹; Robert Kelly²; Eric Schindelholz³; ¹Sandia National Laboratories; ²University of Virginia; ³The Ohio State University

8:50 AM Invited

Melt Pool Boundaries and the Corrosion of Laser Powder Fusion Stainless Steels: *Eric Schindelholz*¹; Michael Melia²; Christopher Barr³; Bradley Jared³; Jeffrey rodelas³; Paul Kotula³; ¹Ohio State University; ²Sandia National Laboratories; ³Sandia National Laboratories

9:20 AM Invited

Selective Corrosion and Sensitization Behavior in Laser Powder Bed Fusion 316L: *Robert Kelly*¹; Duane Macatangay¹; Jenna Conrades¹; Keegan Brunner¹; ¹University of Virginia

9:50 AM

High Performance AM Stainless Steel 316L Under Corrosive Environment: Thomas *Voisin*¹; Zhen Qi¹; Yuliang Zhang¹; Rongpei Shi¹; Josh Kacher²; Manyalibo Matthews¹; Brandon Wood¹; Y. Morris Wang¹; ¹Lawrence Livermore National Laboratory; ²Georgia Tech

10:10 AM

Improving the Corrosion Performance of Additively Manufactured 316L via



THURSDAY AM

TABLE

P

ONTENTS

Chemically-modified Feedstock: Joseph Sopcisak¹; Steven Storck¹; Rengaswamy Srinivasan¹; Jason Trelewicz²; David Sprouster²; Kevin Hemker³; Mo-Rigen He³; Timothy Montalbano¹; ¹Johns Hopkins University Applied Physics Laboratory; ²Stony Brook University; ³Johns Hopkins University

10:30 AM

Electrochemical Response of Additively Printed Inconel 718 by Laser-based **Direct Energy Deposition**: Sangram Mazumder¹; Mangesh V. Pantawane¹; Yee-Hsien Ho¹; Narendra B. Dahotre¹; ¹University of North Texas

10:50 AM

Corrosion Behavior of Functionally Graded Inconel 718 Produced by Additive Manufacturing: Yaiza Gonzalez-Garcia¹; Lola Devignes²; Aytac Yilmaz¹; Arjan de Groot¹; Evgenii Borisov³; Vera Popovich¹; ¹Delft University of Technology; ²SIGMA Clermont; ³Peter de Great Saint-Petersburg Polytechni University

11:10 AM

Nano-crystalline Cold Spray Coatings for Repair and Retrofit of Existing Large-Scale Structures: Rose Roy¹; Baillie Haddad¹; Kris Klus¹; Christian Widener¹; ¹VRC Metal Systems

11:30 AM Invited

Tailoring Microstructure in Additively Manufactured Stainless Steels for Enhanced **Corrosion Performance**: *Jason Trelewicz*¹; David Sprouster¹; Gary Halada¹; Joseph Sopcisak²; Steven Storck²; ¹Stony Brook University; ²The Johns Hopkins University Applied Physics Laboratory

CORROSION

Environmentally Assisted Cracking: Theory and Practice – Environmental

TMS

Embrittlement, Fracture, and Fatigue

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Thursday AM March 18, 2021

Session Chairs: Jian Luo, University of California, San Diego; Stephen Raiman, Texas A&M University

8:30 AM Invited

Corrosion, Irradiation, and Cracking Studies in Support of Coating Development for SiC-based Accident Tolerant Fuel Cladding: *Stephen Raiman*¹; Peter Doyle²; Peter Mouche³; Yutai Katoh³; ¹Texas A&M University; ²University of Tennessee; ³Oak Ridge National Laboratory

9:10 AM

Modeling of Corrosion Crack Dynamics and Fracture Using a Physics-based Meshless Peridynamics Approach: *Srujan Rokkam*¹; Masoud Behzadinasab²; Max Gunzburger³; Sachin Shanbhag³; Nam Phan⁴; ¹Advanced Cooling Technologies Inc; ²Brown University; ³Florida State University; ⁴Naval Air Systems Command

9:30 AM

Humidity and Chemistry Dependent Embrittlement in the Al-Ga-In Liquid Metal Embrittlement System

: *Justin Norkett*¹; Cameron Frampton¹; Victoria Miller¹; ¹University of Florida



9:50 AM

The Effect of Additive Manufacturing Process Parameters on the Fatigue Crack Growth Rates of Alloy 718 in Elevated-pressure and Elevated temperature Hydrogen Gas: *William Hickey*¹; John Macha¹; Vinicio Ynciarte²; Brendy Rincon Troconis²; ¹Southwest Research Institute; ²University of Texas at San Antonio

10:10 AM

Influence of Hydrogen on Softened HAZ during In-situ Slow Strain Rate Testing in YS 550 MPa Grade Steel Welds: *Namhyun Kang*¹; Hanji Park¹; Cheolho Park²; Junghoon Lee²; Stephen Liu³; Dae-Geun Nam⁴; ¹Pusan National University; ²Chosun University; ³Colorado School of Mines; ⁴Korea Institute of Industrial Technology

10:30 AM

Hydrogen Permeability for Determining Hydrogen Embrittlement Susceptibility of High Hardness Steels: *William Williams*¹; David Salley¹; Haley Doude¹; David Wipf¹; Daniel Field²; Krista Limmer²; Kevin Doherty²; Hongjoo Rhee¹; ¹Mississippi State University, CAVS; ²CCDC Army Research Laboratory

10:50 AM

Characterization of Hydrogen Embrittlement Sensitivity of Various High Hardness Steels: David Salley¹; Will Williams¹; Haley Doude¹; Wilburn Whittington¹; Dan Field²; Krista Limmer²; Kevin Doherty²; Hongjoo Rhee¹; *Shiraz Mujahid*³; ¹Center for Advanced Vehicular Systems, Mississippi State University; ²Metals Branch, US CCDC Army Research Laboratory; ³Mississippi State University

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and Computational Modeling — Multiscale Modeling Approaches to Improve

TMS



Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear, University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara

Thursday AM March 18, 2021

Session Chair: Antonios Kontsos, Drexel University

8:30 AM

Experimental Analysis and Numerical Simulation of Cyclic Deformation and Fatigue Behavior of AZ31 Mg Alloy: Abbas Jamali¹; Meijuan Zhang²; Anxin Ma²; Javier Llorca¹; ¹IMDEA Materials Institute & Technical University of Madrid; ²IMDEA Materials Institute

8:50 AM

PRISMS-fatigue: A General Framework for Fatigue Analysis in Polycrystalline the Crystal Plasticity Finite Element Method: Metals and Alloys Using Mohammadreza Yaghoobi¹; Krzysztof S. Stopka²; Aaditya Lakshmanan¹; John E. Allison¹; Veera Sundararaghavan¹; David L. McDowell²; ¹University of Michigan; ²Georgia Institute of Technology

MOBILE-FRIENDL

9:10 AM

Propagation of Microstructure-induced Fatigue Variability onto Stress **Concentrations**: *Gustavo Castelluccio*¹; Farhan Ashraf¹; ¹Cranfield University

9:30 AM

OriginofLong-rangeInternalStresswithHeterogeneousDislocationDistributions: *Yejun Gu*¹; Jaafar El-Awady¹; ¹Johns Hopkins University

9:50 AM

A Simplified Formula to Estimate the Size of the Cyclic Plastic Zone in Metals **Containing Elastic Particles**: *Tito Andriollo*¹; Varvara Kouznetsova²; ¹Technical University of Denmark; ²Eindhoven University of Technology

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Modeling: Process & Properties

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St. Petersburg Polytechnic University

Thursday AM March 18, 2021

Application of Machine Learning for Prediction of Microstructure and Mechanical **Performances in Solid-state Joining Processes**: Benjamin Klusemann¹; Frederic

Bock¹; Uceu Suhuddin¹; Lucian Blaga¹; *Jorge dos Santos*¹; ¹Helmholtz-Zentrum Geesthacht

8:50 AM

Friction Stir Welding Defect Prediction Using Computational Solid Mechanic's Modeling: *Rafael Giorjao*¹; Julian Avila²; Eduardo Monlevade³; Antonio Ramirez¹; Andre Tschiptschin³; ¹The Ohio State University; ²UNESP; ³USP

9:10 AM

The Development of FSW Process Modelling for Use by Process Engineers: *Mike Lewis*¹; Simon Smith²; ¹FTS Engineering Answers Ltd.; ²Transforming Stress Ltd.

9:30 AM

Effect of Tool Geometries on "Heat-input" during Friction Stir Welding of Aluminum Alloys: *Yutaka Sato*¹; Yuichiro Tanai¹; Tianbo Zhao¹; Dalong Yi²; ¹Tohoku University; ²Tsinghua University/Tohoku Univdersity

9:50 AM

Experimental and Numerical Investigations of High Strain Rate Torsion Tests of Al-based Alloys at Elevated Temperatures: *Anton Naumov*¹; Anatolii Borisov¹; Anastasiya Borisova¹; ¹Peter the Great St. Petersburg Polytechnic University

10:10 AM

Numerical Simulation and Analysis of Solid Phase Processing: A Validated Friction Extrusion Smoothed Particle Hydrodynamics Model: Lei Li¹; Xiao Li¹; Anthony Reynolds²; Glenn Grant¹; *Ayoub Soulami*¹; ¹Pacific Northwest National Laboratory; ²University of South Carolina CONTENTS

TABLE

P

Effect of Temperature and Strain Parameters of High Strain Rate Torsion Tests on the Microstructure Evolution of Al-based Alloys: Anastasiya Borisova¹; Elizaveta Anhimova¹; Oleg Zotov¹; *Anton Naumov*¹; Anatolii Borisov¹; ¹Peter the Great St. Petersburg Polytechnic University

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Processing, Defects & Segregation / Steel & Cast Iron

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Thursday AM March 18, 2021

Session Chairs: Hideyuki Yasuda, Kyoto University; Melis Serefoglu, Koç University; Joseph McKeown, Lawrence Livermore National Laboratory; Damien Tourret, IMDEA Materials

8:30 AM

Cellular Automaton Modeling of Solidification Microstructure and Microporosity in Multi-component Aluminum Alloys: Cheng Gu¹; Michael Moodispaw¹; Colin Did governation Algent August 10 bio State Luniversity

Ridgeway¹; *Alan Luo*¹; ¹Ohio State University

Effects of Process Conditions and Morphology Evolution on Microsegregation During Solidification: A Combined Phase-field and Experimental Study: *Zhenjie Yao*¹; David Montiel¹; Mei Li²; Katsuyo Thornton¹; John Allison¹; ¹University of Michigan; ²Ford Motor Company

9:10 AM

Effect of Vacuum during Flow in High-pressure Die Casting: Water Analog Experiments: *Nicole Trometer*¹; Xuejun Huang¹; Emre Cinkilic¹; Alan Luo¹; ¹The Ohio State University

9:30 AM Invited

Grain Selection after a Massive-like Transformation from Ferrite to Austenite during Solidification in Fe-based Alloys: *Hideyuki Yasuda*¹; Taka Narumi¹; Takeru Suga¹; Yukihiko Nanri¹; ¹Kyoto University

10:00 AM

Synchrotron Examination of Nucleation and Growth of Nodular and Compacted Graphite Particles during Cyclic Solidification of Ductile Cast Iron: *Chaoling Xu*¹; Tim Wigger²; Mohammed Azeem³; Tito Andriollo¹; Samuel Clark²; Robert Atwood⁴; Jesper Hattel¹; Peter Lee²; Niels Tiedje¹; ¹Technical University of Denmark; ²University College London, Mechanical Engineering; ³University of Leicester; ⁴Diamond Light Source

10:20 AM

In Situ Quantification of Degenerate Graphite Nodule Formation during the Solidification of Ductile Cast Iron: *Tim Wigger*¹; Tito Andriollo²; Mohammed Azeem³; Chaoling Xu²; Samuel Clark¹; Robert Atwood⁴; Niels Tiedje²; Peter Lee¹; ¹UCL; ²DTU; ³University of Leicester; ⁴Diamond Light Source



SPECIAL TOPICS

Frontiers of Materials Award Symposium: Radiation Processing of Materials — Session I: Radiation Synthesis and Processing of Materials

Program Organizer: Jessika Rojas, Virginia Commonwealth University

Thursday AM March 18, 2021

8:30 AM

Introductory Comments: Frontiers of Materials Award Symposium: Radiation Processing of Materials: *Jessika Rojas*¹; ¹Virginia Commonwealth University

8:35 AM Keynote Ionizing Radiation in the Synthesis and Processing of Nanocomposites for Medical and Environmental Applications: *Jessika Rojas*¹; ¹Virginia Commonwealth University

9:05 AM Invited Radiation-grafting of Smart Polymers for Potential Biomedical Applications: *Emilio Bucio*¹; ¹Nuclear Science Institute at National University of Mexico

9:35 AM Invited Direct Prompt Synthesis of Radioactive Nanoparticles (Prompt Nano Radioisotopes): Carlos Castano¹; ¹Missouri University of Science and Technology

10:05 AM Invited Probing and Processing Nanomaterials and Devices with Radiation: Cory Cress¹;

TMS

¹U.S. Naval Research Laboratory

MOBILE-FRIENDL

NIENIS

Q

10:35 AM Invited Nanochannels, Nanowires, and Nanotubes Fabricated by Ion-track Nanotechnology: *María Eugenia Toimil-Molares*¹; ¹GSI Helmholtz Center

11:05 AM Invited Ionizing Radiation Synthesis of Novel Fabrics for Extraction of Uranium from Seawater: *Mohammed Al-Sheikhly*¹; ¹University of Maryland

11:35 AM Live Question and Answer

NANOSTRUCTURED MATERIALS

Functional Nanomaterials: Functional Low-dimensional Materials (OD, 1D, 2D) Driving Innovations in Electronics, Energy, Sensors, and Environmental Engineering and Science 2021 — 1D Materials & Nanostructures

Sponsored by: TMS Functional Materials Division, TMS: Nanomaterials Committee

Program Organizers: Jiyoung Chang, University of Utah; Michael Cai Wang, University of South Florida; Sarah Zhong, University of South Florida; Sun Choi, Korea Institute of Science and Technology; Pei Dong, George Mason University

Thursday AM March 18, 2021

Session Chairs: Sun Choi, Korea Institute of Science and Technology; Jiyoung Chang, University of Utah



THURSDAY AM

8:30 AM Invited

3D Assembled Functional Structures from Crumpled 2D Nanomaterials: *Baoxing Xu*¹; ¹University of Virginia

8:55 AM

Facile Green Synthesis of ZnInS Quantum Dots: Temporal Evolution of Its Optical Properties and Cell Viability against Normal and Cancerous Cells: Samuel Oluwafemi¹; Nkosingiphile Zikalala¹; Sundararajan Parani¹; ¹University of Johannesburg

9:15 AM Invited

Scalable Synthesis of Nanofibers for Energy Storage and Filtration Applications: *Yuepeng Zhang*¹; Devon Powers¹; Byeongdu Lee¹; Erik Dahl¹; Sanja Tepavcevic¹; Peter Zapol¹; Hee Je Seong¹; Ashley Simmons¹; Mark Koziel¹; Michael LeResche¹; Krzysztof Pupek¹; Gregory Krumdick¹; ¹Argonne National Laboratory

9:40 AM

Growth Mechanism Study of Boron Carbide Nanowires: *Manira Akter*¹; Terry Xu²; ¹University of North Carolina, Charlotte; ²UNCC

10:00 AM

Unveiling the Origin of Morphological Instability in Topologically Complex Electrocatalytic Nanostructures: *Ian Mccue*¹; Yawei Li²; Zhiyong Xia¹; Joshua Snyder³; ¹Johns Hopkins Applied Physics Laboratory; ²National Renewable Energy Laboratory; ³Drexel University

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Alloy

TMS

Development and Application IV

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

March 18, 2021 Thursday AM

Session Chairs: Wei Chen, Illinois Institute of Technology; Jian Luo, University of California, San Diego

8:30 AM Invited From High-entropy Ceramics (HECs) to Compositionally Complex Ceramics (CCCs): Jian Luo¹; ¹University of California, San Diego

8:55 AM

Direct Production of High Entropy Alloy Powders: Jawad Haidar¹; ¹Kinaltek Pty Ltd.

9:15 AM

Hierarchical Eutectoid Nano-lamellar Decomposition in an AlO.3CoFeNi Complex **Concentrated Alloy**: *Sriswaroop Dasari*¹; Bharat Gwalani¹; Abhishek Sharma¹; Vishal Soni¹; Abhinav Jagetia¹; Stephane Gorsse²; Rajarshi Banerjee¹; ¹University of North Texas; ²University of Bordeaux, France



MOBILE-FRIEND

9:35 AM Invited

Data-driven Design of Refractory High-entropy Alloys: Wei Chen¹; George Kim¹; Chanho Lee²; Peter Liaw²; ¹Illinois Institute of Technology; ²University of Tennessee

10:00 AM

Accelerated Alloy Development and Characterization of Compositionally Complex Alloys via High-throughput Methods: Phalgun Nelaturu¹; Michael Moorehead¹; Thien Duong²; Michael Niezgoda¹; Adrien Couet¹; Kumar Sridharan¹; Santanu Chaudhuri²; Dan Thoma¹; ¹University of Wisconsin; ²Argonne National Laboratory

10:20 AM

Nanostructured Oxide-dispersion-strengthened High-entropy Alloys: Xiang Zhang¹; Fei Wang¹; Xueliang Yan¹; Xing-Zhong Li¹; Khalid Hattar²; *Bai Cui*¹; ¹University of Nebraska-Lincoln; ²Sandia National Laboratories

10:40 AM

A High-throughput Strategy to Study Phase Stability and Mechanical Properties in Nb-Ti-V-Zr: Mu Li¹; Zhaohan Zhang¹; Arashdeep Thind¹; Guodong Ren¹; Rohan Mishra¹; Katharine Flores¹; ¹Washington University in St. Louis

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling - Structures and Characterization III



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Thursday AM March 18, 2021

Session Chairs: Keith Knipling, US Naval Research Laboratory; Jonathan Poplawsky, Oak Ridge National Laboratory

8:30 AM

Analysis of Multi-hit Events in Atom Probe Tomography of Refractory High Entropy Alloys: Patrick Callahan¹; Keith Knipling¹; ¹US Naval Research Laboratory

8:50 AM Invited

Heavy Ion Irradiation Response of AlxFeCrNiMn High Entropy Alloys: Nan Li¹; Di Chen²; Youxing Chen³; Jordan Weaver⁴; Yongqiang Wang¹; Saryu Fensin¹; Stuart Maloy¹; Amit Misra⁵; ¹Los Alamos National Laboratory; ²University of Houston; ³University of North Carolina; ⁴National Institute of Standards and Technology; ⁵University of Michigan

9:15 AM Invited

Understanding Radiation Resistance in High Entropy Alloys Through Atom **Probe Tomography**: *Jonathan Poplawsky*¹; Xing Wang¹; Wei-Ying Chen²; Tengfei Yang³; William Weber¹; Yanwen Zhang¹; ¹Oak Ridge National Laboratory; ²Argonne National Laboratory; ³Hunan University





9:40 AM

Grain-scale Plastic Response of Equiatomic CoCrFeMnNi High-entropy Alloy Using High Energy Diffraction Microscopy: Jerard Gordon¹; Rachel Lim¹; Tony Rollett¹; Darren Pagan²; ¹Carnegie Mellon University; ²Cornell High Energy Sychrotron Source

10:00 AM

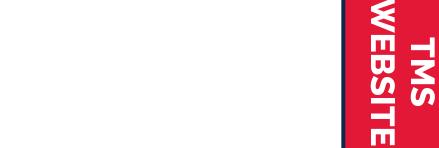
Characteristics of Dislocation Slip in Refractory Multi-principal Element Alloys: *Fulin Wang*¹; Jean-Charles Stinville¹; Marie-Agathe Charpagne¹; Glenn Balbus¹; Leah Mills¹; Tresa Pollock¹; Daniel Gianola¹; ¹University Of California, Santa Barbara

10:20 AM

Nitrogen-induced Solid Solution Hardening of an Austenitic (CrFeMnNi) HEA: *Mathieu Traversier*¹; Pierre Rinn¹; Emmanuel Rigal²; Anna Fraczkiewicz¹; ¹École des mines de Saint-Étienne; ²CEA LITEN

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and Beyond — Superalloys and Beyond: Oxidation and Mechanical Behavior I



Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Thursday AM March 18, 2021

8:30 AM

Early Stage Oxidation of Ni- and Co-based Superalloys: Novel Insights from Rapid ThermalAnnealing (RTA) Experiments: Dorota Kubacka¹; Erdmann Spiecker¹; ¹FAU **Erlangen-Nuremberg**

8:50 AM

Residual Stress with High Temperature Oxidation of Ni-based Haynes 282 **Superalloy**: *Kuan-Che Lan*¹; Hsiao-Ming Tung²; ¹National Tsing Hua University; ²Institute of Nuclear Energy Research

9:10 AM

Understanding the High-temperature Fatigue Properties of the Novel Fe-Ni-Cr Based Superalloy: Shivakant Shukla¹; Govindarajan Muralidharan²; Lawrence Allard²; Jonathan Poplawsky²; ¹Oak Ridge National Laboratory; ²ORNL

9:30 AM

MOBILE-FRIEND

Low Cycle Fatigue of Single Crystal Co- and CoNi-base Superalloys: The Role of Oxidation Resistance: Sean Murray¹; Alice Cervellon¹; Jean-Charles Stinville¹; Jonathan Cormier²; Tresa Pollock¹; ¹University Of California, Santa Barbara; ²ISAE-**ENSMA & Institut Pprime**

9:50 AM

Concomitant Oxidation-diffusion-creep Processes for Stress Generation and Its Effects in Cyclic Oxidation Behavior: Yanfei Gao¹; ¹University of Tennessee -Knoxville

10:10 AM

Effect of Water Species on Formation of Cationic Defects in Yttria-stabilized-Zirconia (YSZ): Amir Saeidi¹; Daniel Mumm¹; ¹University of California, Irvine

10:30 AM

Paving the Way Beyond Ni-based Superalloys: Role of Coupled Thermodynamickinetic Models: *Rishi Pillai*¹; Bruce Pint¹; ¹Oak Ridge National Laboratory

10:50 AM Invited Development of Refractory Metal 'BCC-superalloys' Reinforced by Ordered-BCC Intermetallic Precipitates: Alexander Knowles¹; ¹University of Birmingham

11:20 AM Invited BeyondSuperalloys:AnEfficientStrategyforAssessingEnvironmentalResistance: *Bruce Pint*¹; ¹Oak Ridge National Laboratory

CHARACTERIZATION

Mechanical Response of Materials Investigated through Novel In-situ **Experiments and Modeling — Session VII**



Sponsored by: TMS Structural Materials Division, TMS: Thin Films and Interfaces Committee, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Saurabh Puri, Microstructure Engineering; Amit Pandey, Lockheed Martin Space; Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization; Dongchan Jang, KAIST; Jagannathan Rajagopalan, Arizona State University; Josh Kacher, Georgia Institute of Technology; Minh-Son Pham, Imperial College London; Robert Wheeler, Microtesting Solutions LLC; Shailendra Joshi, University of Houston

Thursday AM March 18, 2021

Session Chair: Dhriti Bhattacharyya, Australian Nuclear Science and Technology Organization

8:30 AM Keynote Microstructural Influences on Grain Boundary Sliding in High Purity Aluminum: *Marissa Linne*¹; Thomas Bieler²; Samantha Daly³; ¹University of Michigan; Lawrence Livermore National Laboratory; ²Michigan State University; ³University of California at Santa Barbara

9:10 AM

In-situ Analysis of Powder Bed Quality during Selective Laser Melting: Tan-Phuc *Le*¹; Matteo Seita¹; ¹Nanyang Technological University

9:30 AM

Non-linear Reversible Behaviour of Metallic Alloys at Low Stresses: Jaji Naveena



*Chamakura*¹; Vera Popovich¹; Jilt Sietsma¹; ¹TU Delft

9:50 AM

Creation of Strength Diagrams of Aluminum Flat Products, Dependent on the Different Thermomechanical Processes: Kaan Ipek¹; Emel Çaliskan²; Derya Dispinar³; ¹Teknik Aluminyum San. A.S.; ²Istanbul University; ³Istanbul Teknik University

10:10 AM

Microscale Insight into the Effect of Twinning on Fracture in a Manganese Steel: *Xinzhu Zheng*¹; Ankit Srivastava¹; ¹Texas A&M University

10:30 AM

Surface Erosion of Spacecraft by High-velocity Regolith Impacts to Simulate Wind Storms on Martian Surfaces: Nicole Bacca¹; Cheng Zhang¹; Arvind Agarwal¹; ¹Florida International University

MATERIALS PROCESSING

Ni-Co 2021: The 5th International Symposium on Nickel and Cobalt — Market, Materials and Mineral Processing



Sponsored by: The Metallurgy & Materials Society of the Canadian Institute of Mining, Metallurgy and Petroleum, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee

Program Organizers: Corby Anderson, Colorado School of Mines; Dean Gregurek, RHI Magnesita; Mari Lundström, Aalto University; Christina Meskers; Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Fiseha Tesfaye, Abo Akademi University; Yuanbo Zhang, Central South University; Sari Muinonen, Glencore; Graeme Goodall, XPS- Glencore; Shijie Wang, Rio Tinto Kennecott Utah Copper Corp (Retired)

Thursday AM March 18, 2021

8:30 AM Invited Global Electrification of Electric Vehicles and Intertwined Material Supply Chains of Cobalt, Copper and Nickel: *Ruby Nguyen*¹; Roderick Eggert²; Corby Anderson; Mike Severson³; ¹Idaho National Laboratory; ²Colorado School of Mines; ³Miami University of Ohio

8:50 AM

AnInnovativeBeneficiationProcessDevelopedforJinchuanNickelOreResources: *Shijie Wang*¹; ¹Rio Tinto Kennecott Utah Copper Corp

9:10 AM Effect of Fluorine on the High Temperature Oxidation Behavior of Nickel-based Alloys: *Alexander Donchev*¹; Mathias Galetz¹; ¹DECHEMA-Forschungsinstitut



ELECTRONIC MATERIALS

Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XX — Advanced Electronic Materials

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Hiroshi Nishikawa, Osaka University; Shih-kang Lin, National Cheng Kung University; Chao-Hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jaeho Lee, Hongik University; Zhi-Quan Liu, Shenzhen Institutes of Advanced Technology; Ming-Tzer Lin, National Chung Hsing University; Dajian Li, Karlsruhe Institute of Technology; Yu Zhong, Worcester Polytechnic Institute; Yee-wen Yen, National Taiwan University of Science and Technology; A.S.Md Abdul Haseeb, University of Malaya; Ligang Zhang, Central South University; Sehoon Yoo, KITECH; Vesa Vuorinen, Aalto University; Yu-chen Liu, National Cheng Kung University

Thursday AM March 18, 2021

Session Chairs: Vuorinen Vesa, Aalto University; Hiroshi Nishikawa, Osaka University

8:30 AM Keynote Solid-LiquidInterdiffusion(SLID)Bonding;ForThermalChallengesinMicrosystem Bonding: *Knut Aasmundtveit*¹; Hoang-Vu Nguyen¹; ¹University of South-Eastern

TMS



Phase Transformations and Microstructural Evolution — General Topic I

9:10 AM Invited

Change in Electric Resistance of Conductive Pastes Including Ag Particles Coated with Various Higher Fatty Acids during Curing Process: *Shinji Fukumoto*¹; Kazuhiro Makimoto¹; Kengo Ohta¹; Yoshihiro Kashiba¹; Michiya Matsushima²; Kozo Fujimoto¹; ¹Osaka University; ²Osaka University

9:40 AM

IMC-freeLow-temperatureTLPCu-to-CuInterconnectionwithExcellentThermal Stability: Shih-kang Lin¹; Yu-chen Liu¹; Chih-han Yang¹; Yu-Hsiang Hsieh¹; Chienwei Huang¹; Chih-feng Lin¹; ¹National Cheng Kung University

10:00 AM

Intermetallic Reactions and Interfacial Stability in Cu-Co-Sn System: Fahimeh Emadi¹; Vesa Vuorinen¹; Hongqun Dong¹; Mervi Paulasto-Kröckel¹; ¹Aalto University

10:20 AM

Synthesis and Characterization of Silver Tin Alloy Powders by High Energy Ball Milling: *Wei-Chen Huang*¹; Chin-Hao Tsai¹; C. Robert Kao¹; ¹National Taiwan University

10:40 AM

Interfacial Microstructure Evolution of Ag/ENIG and Ag/Cu Joint under Thermal Aging: *Min-Su Kim*¹; Sehoon Yoo¹; Hiroshi Nishikawa²; ¹Korea Institute of Industrial Technology; ²Osaka University

PHYSICAL METALLURGY



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Thursday AM March 18, 2021

Session Chair: Qi An, University of Nevada, Reno

8:30 AM

About the Plasticity of Cobalt upon Phase Transformation: A High Temperature Nanoindentation Study: Verena Maier-Kiener¹; Johann Kappacher¹; Helmut Clemens¹; ¹Montanuniversitaet Leoben

8:50 AM

Atomistic Modeling of the Twinning fcc/bcc Phase Transformation in Binary Systems: Quasi-particle Approach and Experiment: *Gilles Demange*¹; Helena Zapolsky²; Kaixuan Chen³; Renaud Patte¹; Zidong Wang³; Pavel Korzhavyi⁴; ¹CNRS-University Of Rouen Normandy; ²Cnrs-University Of Rouen Normandy; ³University of Science and Technology Beijing; ⁴ KTH - Royal Institute of Technology

9:10 AM

Data Assimilation-based Approach to Estimate Grain Boundary Properties Using Phase-field Grain Growth Simulations: *Eisuke Miyoshi*¹; Tomohiro Takaki¹; Yasushi

Shibuta²; Munekazu Ohno³; ¹Kyoto Institute of Technology; ²The University of

Tokyo; ³Hokkaido University

Effects of Oxygen Interstitials on Phase Transformation Paths in Nb-Ti Alloys: *Ravit Silverstein*¹; Raphaële Clément¹; Carlos Levi¹; ¹University of California, Santa Barbara

9:50 AM

In Situ Transformations during Heating of Copper-intercalated Bismuth Telluride: *Pralav Shetty*¹; Matthew McDowell¹; ¹Georgia Institute of Technology

10:10 AM Intrinsic Coupling between Phase Transformation and Deformation Twinning: *Yipeng Gao*¹; ¹The Ohio State University

ELECTRONIC MATERIALS

Recent Advances in Functional Materials and 2D/3D Processing for Sensors, Energy Storage, and Electronic Applications — Functional Materials and 2D/3D Devices

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Pooran Joshi, Oak Ridge National Laboratory; Rahul Panat, Carnegie Mellon University; Ravindra Nuggehalli, New Jersey Institute of Technology; Tolga Aytug, Oak Ridge National Laboratory; Yong Lin Kong, University of Utah; Konstantinos Sierros, West Virginia University



Thursday AM March 18, 2021

Session Chairs: Rahul Panat, Carnegie Mellon University; Tolga Aytug, Oak Ridge National Laboratory; Yong Lin Kong, University of Utah

8:30 AM Invited Additive Manufacturing of NdFeB Bonded Permanent Magnets: Prospects and Challenges: Mariappan Paranthaman¹; ¹Oak Ridge National Laboratory

8:55 AM Invited

Copper-carbon Nanotube Composites Enabled by Electrospinning for Advanced Conductors: *Kai Li*¹; Michael McGuire¹; Andrew Lupini¹; Lydia Skolrood¹; Fred List¹; Burak Ozpineci¹; Soydan Ozcan¹; Tolga Aytug¹; ¹Oak Ridge National Laboratory

9:20 AM

Performance of Chromium Doped Zinc Selenide Nanocrystals: Morphological and Fluorescence Characteristics: *Narsingh Singh*¹; Ching Hua Su¹; Bradley Arnold¹; Fow-Sen Choa¹; David Sachs¹; Brett Setera¹; Christopher Cooper¹; Brian Cullum¹; Kamdeo Mandal¹; ¹University of Maryland, Baltimore County

9:40 AM Invited

Revealing Meso-structure Dynamics in Additive Manufacturing of Energy Storage via Operando Coherent X-ray Scattering: Cheng-Hung Lin¹; Karol Dyro¹; Olivia Chen¹; Dean Yen¹; Bingqian Zheng¹; Surita Bhatia¹; Ke Sun¹; Qingkun Meng²; Lutz Wiegart³; *Yu-chen Karen Chen-Wiegart*⁴; ¹Stony Brook University; ²China University of Mining and Technology; Stony Brook University; ³Brookhaven National Laboratory; ⁴Stony Brook University; Brookhaven National Laboratory

10:05 AM Invited

Sterilize and Recharge Masks Simultaneously for Safe Reuse: Ying Zhong¹; Sriram





NUCLEAR MATERIALS



TENTS

Π

Q

Thermal Property Characterization, Modeling, and Theory in Extreme Environments — Nuclear Fuel Performance & Advanced Thermal Analysis

Sponsored by: TMS Structural Materials Division, TMS: Nuclear Materials Committee

Program Organizers: Janelle Wharry, Purdue University; Mukesh Bachhav, Idaho National Laboratory; Marat Khafizov, Ohio State University; Eric Lass, University of Tennessee-Knoxville; Vikas Tomar, Purdue University; Tiankai Yao, Idaho National Laboratory; Cody Dennett, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Thursday AM March 18, 2021

Session Chairs: Janelle Wharry, Purdue University; Elizabeth Sooby Wood, University of Texas at San Antonio

8:30 AM Ultra-high Lattice Thermal Conductivity and the Effect of Pressure in Superhard Hexagonal BC2N: Safoura Nayeb Sadeghi¹; S. Mehdi Vaez Allaei²; Mona Zebarjadi¹; *Keivan Esfarjani*¹; ¹University of Virginia; ²University of Tehran

8:50 AM Invited Performance of UO2 Reactor Fuel with High Thermal Conductivity Additives: *Michael Tonks*¹; Floyd Hilty¹; ¹University of Florida

9:20 AM Invited Atmosphere Controlled Thermogravimetric Analysis as a Tool to Screen, Test and Qualify Advanced Fuels under Extreme Conditions: *Elizabeth Sooby*¹; ¹University of Texas at San Antonio

9:50 AM

Thermal Stability of Metallic Multilayers with TripleJjunctions: *Tongjun Niu*¹; Yifan Zhang¹; Jaehun Cho¹; Jin Li¹; Haiyan Wang¹; Xinghang Zhang¹; ¹Purdue University

10:10 AM

Energy Balance Investigation of Close-coupled Optimized-pressure Gas Atomization Pour-tube Design Geometry to Prevent Melt Freeze-off: *Franz Hernandez*¹; Eric Deaton¹; Iver Anderson¹; ¹Ames Laboratory of US DOE

NUCLEAR MATERIALS

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — Irradiation Effect in Nuclear Fuels and Materials

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

VEBSITE

TMS



2:00 PM

Point Defect Capture Characteristics and Stress States of Dislocation Loops in α-zirconium: Jose March-Rico¹; Brian Wirth¹; ¹University of Tennessee Knoxville

2:20 PM

Comparison of Void Swelling in Conventional and Novel HT9 Alloys after High Damage Level Ion Irradiation: *Hyosim Kim*¹; Jonathan Gigax¹; Osman Atwani¹; Stuart Maloy¹; Yongqiang Wang¹; Matthew Chancey¹; Jon Baldwin¹; ¹Los Alamos National Laboratory

2:40 PM

Dislocation Loop Formation in Self-ion Irradiated Ultra-high Purity FeCr Alloys: Yao Li¹; Yajie Zhao¹; Arunodaya Bhattacharya²; Jean Henry³; Steven Zinkle¹; ¹The University of Tennessee, Knoxville; ²Oak Ridge National Laboratory; ³The French Alternative Energies and Atomic Energy Commission

3:00 PM

Effect of Microstructure and Rolling Treatment on Static Recrystallization Behavior in Monolithic U-10Mo Fuel Foils: William Frazier¹; Kyoo Sil Choi¹; Lei Li¹; Zhiie Xu¹; Vineet Joshi¹; Ayoub Soulami¹; ¹Pacific Northwest National Laboratory

3:20 PM

Properties of a Helium Ion Beam Degrader for Implanting SSJ2 Tensile Specimens at the LBL 88-Inch Cyclotron: Sarah Stevenson¹; Adi Ben-Artzy¹; Lee Bernstien²; Peter Hosemann¹; ¹University of California, Berkeley; ²LBL



3:40 PM

Proton Irradiation Induced Microstructural Evolution in Compositionally Graded Type 316L Stainless Steel: Xiang Liu¹; Jingfan Yang²; Miao Song³; Xiaoyuan Lou²; Yongfeng Zhang⁴; Lingfeng He¹; Daniel Schwen¹; ¹Idaho National Laboratory; ²Auburn University; ³University of Michigan; ⁴University of Wisconsin-Madison

4:00 PM

Sink Strength Effect on Bubble Formation in Helium-implanted Nanostructured Ferritic Alloys: Yan-Ru Lin¹; Zhanfeng Yan²; David Hoelzer³; Lizhen Tan³; Steven Zinkle¹; ¹University of Tennessee; ²Peking University; ³Oak Ridge National Laboratory

4:20 PM

Synergistic Irradiation and Ageing Effect on Microstructure and Mechanical **Properties of Grade 92 at ~700C**: Weicheng Zhong¹; Lizhen Tan¹; ¹Oak Ridge National Laboratory

4:40 PM

Dislocation Loop Characterization Using STEM-Contrast Techniques in an Irradiated FCC Alloy: *Pengyuan Xiu*¹; Lumin Wang¹; Kevin Field¹; ¹University of Michigan

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Functional, Energy, and Magnetic Materials — **Advanced Manufacturing of Other Functional Materials**



Sponsored by: TMS Functional Materials Division, TMS: Additive Manufacturing Committee, TMS: Magnetic Materials Committee

Program Organizers: Markus Chmielus, University of Pittsburgh; Sneha Prabha Narra, Worcester Polytechnic Institute; Mohammad Elahinia, University of Toledo; Reginald Hamilton, Pennsylvania State University; Iver Anderson, Iowa State University Ames Laboratory

Thursday PM March 18, 2021

2:00 PM

Inconel-steel Multi-metal-material by Liquid dispersed Metal Powder Bed Fusion: Microstructure, Stress and Property Gradients: Sabine Bodner¹; L.T.G. van de Vorst²; Jakub Zalesak³; Juraj Todt³; Julius Keckes³; Verena Maier-Kiener¹; Bernhard Sartory⁴; Norbert Schell⁵; Jaap Hooijmans⁶; Jaco Saurwalt⁶; Jozef Keckes¹; ¹Montanuniversität Leoben; ²TNO; ³Austrian Academy of Sciences; ⁴Materials Center Leoben GmbH; ⁵Helmholtz-Zentrum Geesthacht ; ⁶Admatec Europe BV

2:20 PM

Meltpool Oxidation and Reduction and Inclusion Evolution during the PBF Type Additive Manufacturing: Durim Eo¹; Seong Gyu Chung¹; Jungwook Cho¹; ¹Pohang University of Science and Technology

2:40 PM

Engineered Interconnected Porosity for Enhanced Functional Devices: Scott *Roberts*¹; Ben Furst¹; Eric Sunada¹; ¹Jet Propulsion Laboratory



ADDITIVE TECHNOLOGIES

Additive Manufacturing: Beyond the Beam II – Novel Solid State Processing

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Paul Prichard, Kennametal Inc.; James Paramore, US Army Research Laboratory; Peeyush Nandwana, Oak Ridge National Laboratory; Nihan Tuncer, Desktop Metal

Thursday PM March 18, 2021

Session Chair: Peeyush Nandwana, Oak Ridge National Lab

2:00 PM

Control of High-temperature Drop-on-demand Metal Jetting Through Numerical Modelling and Experimentation: Negar Gilani¹; Nesma Aboulkhair¹; Marco Simonelli¹; Ian Ashcroft¹; Richard Hague¹; ¹University of Nottingham

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — In Situ Characterisation and Material Response to **Build Processes**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

Thursday PM March 18, 2021

Session Chairs: Katerina Christofidou, The University of Sheffield; Bij-Na Kim, Carpenter Additive

2:00 PM

In Situ Synchrotron Observation of Directed Energy Deposition Additive Manufacturing Process: Yunhui Chen¹; Samuel Clark¹; David Collins²; Sebastian Marussi¹; Thomas Connolley³; Robert Atwood³; Oxana Magdysyuk³; Gavin Baxter⁴; Martyn Jones⁴; Chu Lun Alex Leung¹; Peter Lee¹; ¹University College London; ²The University of Birmingham; ³Diamond Light Source; ⁴Rolls-Royce plc

2:20 PM

In-situ TEM Solid-state Thermal Cycling of a Stainless Steel Fabricated via AM: Manas Upadhyay¹; Lluis Yedra-Cardona²; Eva Héripré³; Simon Hallais¹; Alexandre Tanguy¹; ¹LMS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris; ²MSSMat and SPMS, CNRS, CentraleSupeléc, Université Paris-Saclay; ³MSSMat,



CNRS, CentraleSupeléc, Université Paris-Saclay

2:40 PM

Time-resolved Synchrotron X-ray Diffraction Studies of Phase Evolution in Ni alloy 718 during Laser Melting: *Seunghee Oh*¹; Rachel Lim¹; Joseph Aroh¹; Joseph Pauza¹; Andrew Chuang²; Benjamin Gould²; Joel Bernier³; Tao Sun⁴; Robert Suter¹; Anthony Rollett¹; ¹Carnegie Mellon University; ²Argonne National Laboratory; ³Lawrence Livermore National Laboratory; ⁴University of Virginia

3:00 PM

The Effects of Scanning Strategy on Cracking and Grain Structure of the IN738LC Superalloy Produced by Selective Laser Melting: *Marcus Lam*¹; ¹Monash University

3:20 PM

Aging Effects on Phase Transformation and Microstructure Evolution in Selective Laser Melted NiTi Shape Memory Alloy: *Madhavan Radhakrishnan*¹; Sayed Saghaian²; Mohammadreza Nematollahi³; Keyvan Safaei³; Osman Anderoglu¹; Mohammad Elahinia³; Haluk Karaca²; ¹University of New Mexico; ²University of Kentucky; ³University of Toledo

3:40 PM

Study of the Role of Beam Scan Strategies on the Microstructure and Mechanical Properties of EBM Additively Manufactured Ti-6Al-4V Builds: *Meiyue Shao*¹; Sriram Vijayan¹; Sabina Kumar²; Sudarsanam Babu²; Joerg Jinschek¹; ¹The Ohio State University; ²University of Tennessee

4:00 PM

Microstructural Control and Refinement in DMLS Ti-6Al-4V: *Matthew Vaughn*¹; Justin Unger¹; Matthew Dunstan²; Andrew Gaynor²; Brandon Mcwilliams²; James Guest¹; Kevin Hemker¹; ¹Johns Hopkins University; ²Army Research Laboratory





Advanced Functional and Structural Thin Films and Coatings — Thin Films and **Nanostructures for Optoelectronics II**

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

Thursday PM March 18, 2021

Session Chairs: Ramana Chintalapalle, UTEP; Gerald Ferblantier, ICUBE

2:00 PM Keynote Metamaterial Coatings for Tuning Optical and Fluid Wetting Behavior: Shawn *Putnam*¹; ¹University of Central Florida

2:45 PM

Simulation of Optical Properties for Multilayers from Extreme Ultraviolet to Far Infrared: Legi Lin¹; Nuggehalli Ravindra¹; ¹New Jersey Institute of Technology

3:05 PM Invited Localization of Dopants and Optical Properties of Phosphorus Doped Silicon Nanocrystals: *Hervé Rinnert*¹; Alaa Eldin Giba¹; Fatme Trad¹; Mathieu Stoffel¹; Xavier Devaux¹; Alexandre Bouché¹; Michel Vergnat¹; Rémi Demoulin²; Etienne Talbot²; Anne-Sophie Royet³; Pablo Acosta Alba³; Sébastien Kerdiles³; ¹University of Lorraine, IJL; ²Université de Rouen, GPM; ³Université Grenoble Alpes, CEA

3:40 PM

Interface Characteristics in Transparent Optical Nanomultilayers: Danielle White¹; Chelsea Appleget¹; Andrea Hodge¹; ¹University of Southern California

4:00 PM

Pulsed-laser Deposition and Optical Characterization of Gallium Oxide (Ga₂O₃) Thin Films: Vishal Zade¹; Nanthkishore Makeswaran¹; Ramana Chintalapalle¹; ¹UTEP

ENERGY & ENVIRONMENT

Advanced Magnetic Materials for Energy and Power Conversion Applications - Advances in Characterization, Processing, and Design of Magnetic Materials

Sponsored by: TMS Functional Materials Division, TMS: Magnetic Materials Committee

Program Organizers: Richard Beddingfield, North Carolina State University; Daniel Salazar, BCMaterials; Alex Leary, NASA Glenn Research Center; Huseyin Ucar, California Polytechnic University; Yongmei Jin, Michigan Technological University; Arcady Zhukov, University of the Basque Country

March 18, 2021 **Thursday PM**

Session Chair: Daniel Salazar, BCMaterials

2:00 PM Invited



THURSDAY PM

ONTENTS FABLE OF

2:30 PM A Refinement Program to Characterize Single Crystal Magnetic Diffuse Scattering from Neutron Diffraction Experiments: Zachary Morgan¹; Feng Ye²; ¹Michigan Technological University; ²Oak Ridge National Laboratory

2:50 PM

Scale-up Production on MnBi Magnet with High Performance: Wei Tang¹; Gaoyuan Ouyang¹; Xubo Liu¹; Baozhi Cui¹; Kevin Dennis¹; Jun Cui²; ¹Ames Laboratories; ²Iowa State University

3:10 PM Invited Exchange-coupled Ferromagnetism in Self-assembled Co-Pt Nanochessboards: Jerrold Floro¹; ¹University of Virginia

3:40 PM Invited Neutron Diffraction: A Key Tool to Unravel the Magnetic Behaviour in Heusler Alloys: Jose Maria Porro¹; ¹BCMaterials & Ikerbasque

4:10 PM

Magnetic Field-assisted HDDR Processing of NdFeB Powders: Michael Kesler¹; Xubo Lui²; Ikenna Nlebedim²; Matthew Kramer²; Michael McGuire¹; ¹Oak Ridge National Laboratory; ²Ames Laboratory

4:30 PM

Magnetic Domain Observation by Soft X-ray Magnetic Circular Dichroism Microscopy of Nd-Fe-B-Ga Sintered Magnets Under High Magnetic Field and High Temperature: Andres Martin-Cid¹; Shintaro Kobayashi²; David Billington²; Kentaro Toyoki²; Yoshinori Kotani²; Yukio Takada³; Takashi Sato³; Yuji Kaneko³; Akira Kato⁴; Taisuke Sasaki⁵; Tadakatsu Ohkubo⁵; Kazuhiro Hono⁵; Satoshi Hirosawa⁵; Motohiro Suzuki²; Tetsuya Nakamura⁶; ¹Japan Synchrotron Radiation Research Institute (JASRI), SPring-8; ²Japan Synchrotron Radiation Research Institute (JASRI), SPring-8; ³Toyota Central R&D Labs, Inc; ⁴Advanced Material Engineering Division, Toyota Motor Corporation; ⁵National Institute for Materials Science; ⁶Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University



ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII — Energy **Conversion and Storage II**

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Thursday PM March 18, 2021

Session Chairs: Partha Mukherjee, Purdue University; Boniface Fokwa, University of California Riverside

2:00 PM Invited Designing Earth-abundant Boron-based Electrocatalysts for Hydrogen **Production**: Eunsoo Lee¹; Hyounmyung Park¹; Palani Jothi¹; Yuemei Zhang¹; *Boniface Fokwa*¹; ¹University of California, Riverside



Thursday PM March 18, 2021

2:30 PM

Morphology Study of Palladium Produced by Electrodeposition from EMIM-Cl Ionic Liquid: *Wu Zhang*¹; Batric Pesic²; ¹Shenyang Ligong University; ²University of Idaho

2:50 PM Synthetic Control of Nanostructured Bilayered Vanadium Oxides for Intercalation Batteries: *Ekaterina Pomerantseva*¹; ¹Drexel University

3:20 PM

Understanding the Role of Water-soluble Additive and pH in the Fabrication of Directionally Porous Electrodes for Lithium-Ion Batteries: *Rohan Parai*¹; Justine Marin¹; Dipankar Ghosh¹; Ziyang Nie²; Gary Koenig²; ¹Old Dominion University; ²University of Virginia

MATERIALS DESIGN

Advances in Titanium Technology — General Topic of Ti and Ti Alloys

Sponsored by: TMS Structural Materials Division, TMS: Titanium Committee

Program Organizers: Don Li, Howmet Engineered Products; Yufeng Zheng, University of Nevada-Reno ; Peeyush Nandwana, Oak Ridge National Laboratory; Matthew Dunstan, US Army Research Laboratory **NITENIIS**

9



MOBILE-FRIEND

2:00 PM

The Effect of Process Parameters on Abnormal Grain Growth during Beta Annealing of Hot-Forged Ti-6Al-4V: *Nathan Levkulich*¹; Lee Semiatin²; Adam Pilchak²; Eric Payton²; ¹Ues Inc.; ²Air Force Research Laboratory

LIGHT METALS

Aluminum Reduction Technology — Continue Environment (Material and Equipment) & Fundamental Studies (Alumina Dissolution and Bath)

Sponsored by: TMS Light Metals Division, TMS: Aluminum Committee

Program Organizers: Nadia Ahli, Emirates Global Aluminium; Nancy Holt, Hydro Aluminium AS

Thursday PM March 18, 2021

Session Chair: Bertrand Allano, RIO TINTO

2:00 PM

Instant Monitoring of Aluminum Chemistry in Cells Using a Portable Liquid Metal Analyzer: Sveinn Hinrik Gudmundsson¹; Birna Björnsdóttir²; *Kristjan Leosson*¹; ¹DT Equipment; ²Nordural ehf

2:20 PM

Dissolution Characteristics and Concentration Measurements of Alumina in

Cryolite Melts: Luis Bracamonte¹; Vegard Aulie¹; Christian Rosenkilde²; Kristian

Einarsrud¹; Espen Sandnes¹; ¹Ntnu University; ²Hydro Aluminium

BIOMATERIALS

Biological Materials Science — Biological Materials Science IV

2:40 PM

On Gaseous Emissions during Alumina Feeding: *Sindre Engzelius Gylver*¹; Åste Follo²; Vegard Aulie¹; Espen Sandnes¹; Helene Marie Granlund³; Anders Sørhuus⁴; Kristian Etienne Einarsrud¹; ¹Norwegian University of Science and Technology; ²Elkem; ³Alcoa Mosjøen; ⁴GE Power

3:00 PM

On the Feasibility of Using Low-melting Bath to Accommodate Inert Anodes in Aluminium Electrolysis Cells: Asbjorn Solheim¹; ¹SINTEF Industry

3:20 PM

Electrochemical Reduction and Dissolution of Aluminium in a Thin-layer Refinery Process: *Andrey Yasinskiy*¹; Peter Polyakov¹; Ilya Moiseenko¹; Sai Krishna Padamata¹; ¹Siberian Federal University

3:40 PM

Influence of Additives on Alumina Dissolution in Superheated Cryolite Melts: *Jonathan Alarie*¹; László Kiss¹; Sándor Poncsák¹; Renaud Santerre²; Sébastien Guérard³; Jean-François Bilodeau³; ¹University of Quebec at Chicoutimi; ²Technical Advisor, Retired from Rio Tinto; ³Arvida Research and Development Centre, Rio Tinto

4:00 PM Question and Answer Period

5021 2021

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Biomaterials Committee

Program Organizers: David Restrepo, University of Texas at San Antonio; Steven Naleway, University of Utah; Jing Du, Pennsylvania State University; Ning Zhang, University of Alabama

Thursday PM March 18, 2021

Session Chairs: Steven Naleway, The University of Utah; Ning Zhang, The University of Alabama

2:00 PM Invited Understanding Heterogeneity in Bone Adaptation Following Exercise: Mariana Kersh¹; Sony Manandhar¹; Hyunggwi Song¹; John Polk¹; ¹University of Illinois at Urbana-Champaign

2:30 PM

Internal Strain Mapping for Native and Implanted Glenoids: Yuxiao Zhou¹; Gregory Lewis¹; April Armstrong¹; *Jing Du*¹; ¹Penn State University

2:50 PM

Negative Compressibility Architected Materials for Novel Cardiac Patches: *Juan Sebastian Rincon Tabares*¹; David Restrepo¹; Juan Velasquez¹; Hai-Chao Han¹; ¹University of Texas at San Antonio

3:10 PM

Investigating the Effect of Morphological Parameters on the Sound-Induced Mechanical Response of Mosquito Antennae: Adwait A. Trikanad¹; Hoover Pantoja-

Sánchez¹; Ximena Bernal²; Pablo Zavattieri¹; ¹Purdue University; ²Purdue University,

Smithsonian Tropical Research Institute



Q

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII – Alloy Design and Development

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa **Technical Center**

Thursday PM March 18, 2021

Session Chairs: Kefu Yao, Tsinghua University; Qiaoshi Zeng, Center for High Pressure Science and Technology Advanced Research

2:00 PM

Atomistic Characterization and Modeling of Corrosion in Al-based Amorphous **Metals**: *Jia Chen*¹; Wenjun Cai¹; ¹Virginia Polytechnic Institute and State University

2:20 PM

Synthesis of Bulk Metallic Glass-alumina Composites with Intertwined Dendritic Structure: Je In Lee¹; Amy Wat²; Chae Woo Ryu³; Jinyeon Kim³; Eun Soo Park³; Robert Ritchie²; ¹Pusan National University; ²University of California, Berkeley;

NUCLEAR MATERIALS

Ceramic Materials for Nuclear Energy Research and Applications — Advanced **Ceramics Concepts**

Sponsored by: TMS Extraction and Processing Division, TMS Structural Materials Division, TMS Light Metals Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Committee, TMS: Nuclear Materials Committee

Program Organizers: Xian-Ming Bai, Virginia Polytechnic Institute and State University; Yongfeng Zhang, University of Wisconsin-Madison; Larry Aagesen, Idaho National Laboratory; Vincenzo Rondinella, Jrc-Ec

Thursday PM March 18, 2021

Session Chairs: Haiming Wen, Missouri University of Science and Technology; Xunxiang Hu, Oak Ridge National Laboratory

2:00 PM Invited **Development of Yttrium Hydride for High Temperature Moderator Application:** *Xunxiang Hu*¹; Kurt Terrani¹; ¹Oak Ridge National Laboratory

2:30 PM

Ionization Effects on Damage Accumulation Behavior in SiC: Lauren Nuckols¹; Miguel Crespillo¹; Yanwen Zhang²; William Weber¹; ¹University of Tennessee Knoxville; ²Oak Ridge National Laboratory



9

THURSDAY PM

2:50 PM

Microstructural Characterization of Radiation Effects in 3D printed SiC: Timothy Lach¹; Takaaki Koyanagi¹; Chad Parish¹; Thak Sang Byun¹; Kurt Terrani¹; ¹Oak Ridge National Laboratory

3:10 PM Invited Microstructure and Chemical States of Fission Products in Irradiated AGR-1 and AGR-2 TRISO Particle UCO Fuel Kernels: Yong Yang¹; Isabella van Rooyen²; Zhenyu Fu¹; Boopathy Kombaiah²; ¹University of Florida; ²Idaho National Laboratory

3:40 PM Invited **Oxidation Behavior of TRISO Fuel Materials**: *Haiming Wen*¹; Adam Bratten¹; Visharad Jalan¹; ¹Missouri University of Science and Technology

4:10 PM

Evolution of Ion Irradiated Nitride Ceramics Properties for Coated Particle Fuel Systems: Adrien Terricabras¹; Alicia Raftery²; Andrew Nelson²; Steven Zinkle¹; ¹University of Tennessee; ²Oak Ridge National Laboratory

4:30 PM

On the Role of Neutron Irradiation Damages on Fission Products Transport in the SiC Layer of TRISO Fuel Particles: Subhashish Meher¹; Isabella van Rooyen¹; Chao Jiang¹; ¹Idaho National Laboratory

CHARACTERIZATION

Characterization of Materials through High Resolution Imaging — Algorithms for High Resolution Coherent Imaging of Materials



Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee

Program Organizers: Richard Sandberg, Brigham Young University; Ross Harder, Argonne National Laboratory; Xianghui Xiao, Brookhaven National Laboratory; Brian Abbey, La Trobe University; Saryu Fensin, Los Alamos National Laboratory; Ana Diaz, Paul Scherrer Institut; Mathew Cherukara, Argonne National Laboratory

Thursday PM March 18, 2021

Session Chair: Mathew Cherukara, Argonne National Laboratory

2:00 PM Invited **Optimization Based Approach for 3D Alignment in X-ray Nano-tomography:** *Kanupriya Pande*¹; ¹Lawrence Berkeley National Laboratory

2:30 PM

Adaptive Machine Learning for 3D Bragg Coherent Diffraction Imaging **Reconstructions**: Alexander Scheinker¹; Reeju Pokharel¹; ¹Los Alamos National Laboratory

2:50 PM Invited **Exploiting Machine Learning Techniques in X-ray Ptychography**: *Pablo Enfedaque*¹; ¹LBNL

3:20 PM

Ptychographic Inversion with Deep Learning Network and Automatic **Differentiation**: *Tao Zhou*¹; Mathew Cherukara¹; Saugat Kandel¹; Stephan Hruszkewycz¹; Alexander Hexemer¹; Ross Harder¹; Pablo Enfedaque¹; Martin Holt¹;

TMS



3:40 PM

Image-based Simulation of Permeability and Image-to-Mesh Conversion of X-ray Tomographic Images of a Nickel Foam: S. Ali Shojaee¹; Arsalan Zolfaghari¹; ¹Thermo Fisher Scientific

4:00 PM Invited

Using Phase Field Simulations to Train Convolutional Neural Networks for Segmentation of Experimental Materials Imaging Datasets: Tiberiu Stan¹; Jiwon Yeom²; Seungbum Hong²; Peter Voorhees¹; ¹Northwestern University; ²Korea Advanced Institute of Science and Technology

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Metallurgical **Process Optimization**

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory



Session Chairs: Rajiv Soman, Eurofins EAG Materials Science LLC; Arnab Baksi, Merichem Company

2:00 PM

Structure and Magnetic Properties of Gas-atomized Maraging Steel Powders for Additive Manufacturing: Ganesh Varma Thotakura¹; Alex Paul¹; Ramasis Goswami²; *Tanjore Jayaraman*¹; ¹University of Michigan-Dearborn; ²Naval Research Laboratory

2:20 PM

Effects of Sinter Feed Size on Productivity and Quality of Iron Ore Sinter: Mingming Zhang¹; Marcelo Andrade¹; ¹ArcelorMittal Global R&D

2:40 PM

Characterization of Brazilian Linz Donawitz-LD Steel Sludges: Mery Gomez-*Marroquin*¹; Roberto de Avillez²; Sonia Letichevsky²; Dalia Carbonel-Ramos³; Antoni Quintanilla-Balbuena⁴; Kenny Salazar-Yantas⁴; ¹APMMM/UNI; ²DEQM PUC-Rio; ³FIA UNI; ⁴FIGMM UNI

3:00 PM

Manufacture of Porous Frit Vents using Space Holder Methodology for **Radioisotopic Space Power Systems**: *Gareth Sheppard*¹; Karl Tassenburg¹; Ramy Mesalam¹; Bogdan Nenchev¹; Joel Strickland¹; Hugo Williams¹; ¹University of Leicester

ADDITIVE TECHNOLOGIES

Computational Techniques for Multi-Scale Modeling in Advanced Manufacturing — Multiscale Solid-state Models



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Extraction and Processing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, University of Alabama; Mei Li, Ford Motor Company; Alexandra Anderson, Gopher Resource; Srujan Rokkam, Advanced Cooling Technologies Inc

Thursday PM March 18, 2021

Session Chair: Srujan Rokkam, Advanced Cooling Technologies Inc.

2:00 PM Invited Multiscale Crystal Plasticity in Integrated Computational Materials Engineering: Deepankar Pal¹; Javed Akram¹; Thaddeus Song¹; Jobie Gerken¹; Dave Conover¹; ¹Ansys

2:40 PM

Microstructure Based Modeling of Friction Stir Welded Joint between Dissimilar Metals Using Crystal Plasticity: Shank Kulkarni¹; Kyoo Sil Choi¹; Piyush Upadhyay¹; Ayoub Soulami¹; ¹Pacific Northwest National Laboratory

3:05 PM

Modeling Material Behavior during Continuous Bending Under Tension for Inferring the Post-necking Strain Hardening Response of Ductile Sheet Metals: Application to Dual-phase Steels: Marko Knezevic¹; Russell Marki¹; ¹University of **New Hampshire**



3:30 PM

Modeling the Role of Local Crystallographic Correlations in Microstructures of Ti-6Al-4V Using a Lamellar Visco-plastic Self-consistent Polycrystal Plasticity **Formulation**: *Iftekhar Riyad*¹; Ricardo Lebensohn²; Brandon McWilliams³; Adam Pilchak⁴; Marko Knezevic¹; ¹University of New Hampshire; ²Los Alamos National Laboratory; ³CCDC Army Research Laboratory; ⁴Air Force Research Laboratory

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics — Phonons, Magnons and Other **Excitations**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

Thursday PM March 18, 2021

Session Chairs: Chen Li, University of California Riverside; Huajing (Wilson) Song, Los Alamos National Laboratory; Sara Kadkhodaei, University Of Illinois At Chicago; Jorge Munoz, University of Texas El Paso

2:00 PM Invited

Phonons and Transition-induced Plasticity of bcc Refractory High-entropy Alloys from First Principles: Yuji Ikeda¹; Prashanth Srinivasan²; Blazej Grabowski¹;

MOBILE-FRIENDL

Fritz Körmann³; ¹University of Stuttgart; ²TU Delft; ³Max-Planck-Institut für Eisenforschung GmbH; TU Delft

2:30 PM

Contributions of Atom Vibrations to the Heat of Fusion of Germanium: Camille *Bernal*¹; Claire Saunders¹; Stefan H. Lohaus¹; Douglas Abernathy²; Brent Fultz¹; ¹California Institute of Technology; ²Oak Ridge National Laboratory

2:50 PM

A Computational and Experimental Study of Phonon Anharmonicity and Thermal **Expansion of Cuprous Oxide**: *Claire Saunders*¹; Dennis Kim²; Hillary Smith³; Brent Fultz¹; ¹California Institute of Technology; ²Massachusetts Institute of Technology; ³Swarthmore College

3:10 PM Invited

Development of New Ab-initio Non-adiabatic Excited-state Molecular Dynamics Method in NWChem: *Huajing (Wilson) Song*¹; Sean Fischer²; Victor Freixas³; Niranjan Govind⁴; Sergei Tretiak¹; ¹Physics and Chemistry of Materials, Los Alamos National Lab; ²U.S. Naval Research Laboratory; ³Universidad Nacional de Quilmes; ⁴Pacific Northwest National Laboratory

3:40 PM

First Principle Studies of Charged Point Defect in Phosphorene: *Biswas Rijal*¹; Anne Marie Tan¹; Christoph Freysoldt²; Richard Hennig¹; ¹University of Florida; ²Max **Planck Institute**

4:00 PM

Negative Grüneisen Parameters in Nonmagnetic

bcc-based Intermetallic FeTi at High Pressure: Bethuel Khamala¹; Jorge Munoz²; ¹University of Texas El Paso; ²University of Texas El Paso



THURSDAY PM

TABLE OF

4:20 PM Invited Anomalous Magnon-phonon Dynamics in Antiferromagnets: Chen Li¹; ¹University of California Riverside

CORROSION

Environmental Degradation of Additively Manufactured Alloys – Material Degradation in Irradiated Environments, Environmental Assisted Cracking

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee, TMS: Additive Manufacturing Committee

Program Organizers: Kinga Unocic, Oak Ridge National Laboratory; Jenifer Locke, Ohio State University; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Xiaoyuan Lou, Auburn University; Brendy Rincon Troconis, University of Texas at San Antonio; Luke Brewer, University of Alabama

Thursday PM March 18, 2021

Session Chairs: Kinga Unocic, Oak Ridge National Laboratory; Sebastien Dryepondt, Oak Ridge National Laboratory; Michael Kirka, Oak Ridge National Laboratory

2:00 PM Invited Additively Manufactured 316L Stainless Steel for Nuclear Applications: Gary Was¹; *Miao Song*¹; ¹University of Michigan



2:30 PM

Comparison of Oxidation Behavior of Ultrasonic Additively Manufactured and Conventional Zircaloy-4: *Cory Parker*¹; Kenneth Kane¹; Stephen Raiman¹; Bruce Pint¹; Caleb Massey¹; Andrew Nelson¹; ¹Oak Ridge National Laboratory

2:50 PM

Performance of Additively Manufactured FeCrAl Alloy Accident Tolerant Fuel Cladding in Nuclear Power Reactor Environments: Vipul Gupta¹; Andrew Hoffman¹; Raul Rebak¹; ¹GE Research

3:10 PM

Sensitization and Stress Corrosion Cracking of Alloy 800H by Laser Powder Bed Fusion: Jingfan Yang¹; Xiang Liu²; Miao Song³; Lingfeng He²; Xiaoyuan Lou¹; ¹Auburn University; ²Idaho National Laboratory; ³University of Michigan

CORROSION

Environmentally Assisted Cracking: Theory and Practice — Corrosion and **Fracture in Harsh Environments**

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

NTENTS

O



THURSDAY PM

Session Chairs: Nikhilesh Chawla, Purdue University; Brendy Troconis, University of Texas at San Antonio

2:00 PM Invited

Spectroelectrochemical Evaluation of Carbon Steelin Slightly Sour Environments Under the Presence of H₂S/CO₂ and Triazine-Based H₂S Scavenger: Vinicio Ynciarte¹; Leonardo Caseres²; James Dante²; *Brendy Rincon Troconis*¹; ¹University of Texas at San Antonio; ²Southwest Research Institute

2:40 PM

A Multiphysics Model of Synergistic Environmental Exposure Assisted Damage of Composite Using Homogenization-based Degradation Variables: Zhiye Li¹; Michael Lepech¹; ¹Stanford University

3:00 PM

Combined Ab-initio and Experimental Study of Hydrogen Sorption in Dual Phase **Steels**: Saurabh Sagar¹; Vera Popovich¹; Pascal Kömmelt²; Poulumi Dey¹; ¹Delft University of Technology; ²Research and Development, Forming Technology, Tata Steel Ijmuiden BV

3:20 PM

Fatigue Crack Propagation in AA7085-T7451 Exposed to Complex Atmospheric **Environments**: *Brandon Free*¹; Sarah Galyon Dorman²; Jason Niebuhr²; Jenifer Locke¹; ¹The Ohio State Uniersity; ²SAFE Inc.

3:40 PM

The Effect of Applied Potential and Loading Rate on the Hydrogen Environmentassisted Cracking Behavior of AA7075-T6511: Zachary Harris¹; Alen Korjenic¹; John Scully¹; James Burns¹; ¹University of Virginia



4:00 PM

Phase-field Modeling of Galvanic Corrosion in Magnesium-Aluminum Joints: *Kubra Karayagiz*¹; Adam Powell¹; Qingli Ding¹; Brajendra Mishra¹; ¹Worcester **Polytechnic Institute**

4:20 PM

Understanding Pitting Corrosion in a High-performance Aluminum Alloy by Four-dimensional (4D) X-ray Microtomography: Daniel Sinclair¹; Sridhar Niverty¹; Nikhilesh Chawla¹; ¹Purdue University

4:40 PM

Formation of Ni-O-H-S Surface Phases on Cathodically Charged Ni: Lai Jiang¹; Stanislav Verkhoturov¹; Emile Schweikert¹; Michael Demkowicz¹; ¹Texas A&M University

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and **Computational Modeling — Data-Driven Investigations of Fatigue**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear,





University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara

Thursday PM March 18, 2021

Session Chair: Ashley Spear, University of Utah

2:00 PM

Discovering the Structural Signature of Fatigue Crack Growth Rate Using Computer Vision and Machine Learning: Katelyn Jones¹; William Musinski²; Adam Pilchak²; Reji John²; Paul Shade²; Anthony Rollett¹; Elizabeth Holm¹; ¹Carnegie Mellon University; ²Air Force Research Laboratory

2:20 PM

A Microstructural Model for Fatigue in NiTi Shape Memory Alloy Based on Information Fusion from Advanced Experiments and Simulation: Harshad *Paranjape*¹; Darren Pagan²; Sivom Manchiraju³; Peter Anderson⁴; Craig Bonsignore¹; Justin Gilbert¹; Ich Ong¹; Lot Vien¹; ¹Confluent Medical; ²Pennsylvania State University; ³Ansys, Inc.; ⁴The Ohio State University

2:40 PM

In-situ Diffraction and Cohesive-zone Studies of the Fatigue-crack-growth Behavior in the ZK60 Mg Alloy: Di Xie¹; Peter Liaw¹; Yang Ren²; Yanfei Gao¹; ¹University of Tennessee; ²Argonne National Laboratory

MATERIALS PROCESSING

Friction Stir Welding and Processing XI — Spot Technologies



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Yuri Hovanski, Brigham Young University; Piyush Upadhyay, Pacific Northwest National Laboratory; Yutaka Sato, Tohoku University; Nilesh Kumar, University of Alabama, Tuscaloosa; Anton Naumov, Peter the Great St. Petersburg Polytechnic University

Thursday PM March 18, 2021

2:00 PM

Advances in Refill Spot Welding Productivity: Yuri Hovanski¹; Andrew Curtis¹; Sarah Michaelis¹; Paul Blackhurst¹; Brigham Larsen¹; ¹Brigham Young University

2:20 PM

Finite Element Analysis and Failure Mechanisms of Refill Friction Stir Spot Welding: Enkhsaikhan Boldsaikhan¹; Shintaro Fukada²; Mitsuo Fujimoto²; Kenichi Kamimuki²; ¹Wichita State University; ²Kawasaki Heavy Industries, Inc.

2:40 PM

Characterization of Intermetallics Formation in µFSSW of Dissimilar Al/Cu Alloy **Sheets**: *David Yan*¹; Logan Vahlstrom¹; ¹San Jose State University

3:00 PM

Dissimilar Friction Stir Spot Welding of Low Carbon Steel and Aluminum Alloy by **Double Side Adjustable Tools**: *Xiaopei Wang*¹; Yoshiaki Morisada¹; Hidetoshi Fujii¹; ¹Osaka University

TABLE OF

ONTENTS

3:20 PM

Microstructural Characterization of Lap-jointed Ti-6Al-4V Plates by Pin-less Friction Stir Spot Welding: Hyojin Park¹; Yong Chae Lim²; Scott A Rose³; Zhili Feng²; Hahn Choo¹; ¹University of Tennessee, Knoxville; ²Oak Ridge National Laboratory; ³Boeing

3:40 PM

Temperature Distribution during Friction Stir Spot Welding of Thin AA 6082-T6 and AA 5082-0 Sheets: *Mikhail Ozhegov*¹; Fedor Isupov¹; Roman Smelianskii¹; ¹St. Petersburg Polytechnic University of Peter the Great

NANOSTRUCTURED MATERIALS

Functional Nanomaterials: Functional Low-dimensional Materials (OD, 1D, 2D) Driving Innovations in Electronics, Energy, Sensors, and Environmental **Engineering and Science 2021 — Functional Nanomaterials**

Sponsored by: TMS Functional Materials Division, TMS: Nanomaterials Committee

Program Organizers: Jiyoung Chang, University of Utah; Michael Cai Wang, University of South Florida; Sarah Zhong, University of South Florida; Sun Choi, Korea Institute of Science and Technology; Pei Dong, George Mason University

Thursday PM March 18, 2021

Session Chairs: Sarah Zhong, University of South Florida; Michael Wang, University of South Florida



MOBILE-FRIENDL

ONTENTS

TABLE

ę

2:00 PM Invited

Direct Backbone Attachment of Polyesters on Grain Boundaries Enhances ChemicalStabilityandSuppressingIonMigrationinCH₃NH₃Pbl₃HybridPerovskite **Solar Cells**: *Chang-Yong Nam*¹; ¹Brookhaven National Laboratory

2:25 PM

Antireflective Hybrid Nanocoatings Derived via Heated Liquid-phase Infiltration in Hierarchically Self-Assembled Block Copolymer Thin Film Templates: Ashwanth Subramanian¹; Nikhil Tiwale²; Gregory Doerk²; Kim Kisslinger²; Chang-Yong Nam²; ¹Stony Brook University; ²Brookhaven National Laboratory

2:45 PM

Giant Low-temperature Anharmonicity in Silicon Nanocrystals: Shuonan Chen¹; Devin Coleman¹; Douglas Abernathy²; Arnab Banerjee²; Luke Daemen²; Lorenzo Mangolini¹; Chen Li¹; ¹University of California, Riverside; ²Oak Ridge National Laboratory

3:05 PM Invited

Nanomaterials for Multispectral Adaptive Radiative Heating and Cooling: Po-*Chun Hsu*¹; ¹Duke University

3:30 PM Invited

Silicon Carbide Biotechnology: Carbon-based Neural Interfaces: Chenyin Feng¹; Mohamad Beygi¹; Christopher Frewin¹; Md Rubayat-E Tanjil Rubayat-E Tanjil²; Ashok Kumar²; Michael Wang²; *Stephen Saddow*¹; ¹University of South Florida; ²USF ME

3:55 PM

Substituent Effects on Electronic Properties of Cy5: Density Functional and Time-**Dependent Density Functional Calculations**: Austin Biaggne¹; Lan Li¹; Bernard



THURSDAY PM

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Thermal and **Other Properties**

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Thursday PM March 18, 2021

Session Chairs: John Scully, University of Virginia; Gerald Frankel, The Ohio State University

2:00 PM Invited

Controlling the Corrosion Resistance of Multi-principal Element Alloys: John *Scully*¹; Samuel Inman¹; Angela Gerard¹; Christopher Taylor²; Wolfgang Windl²; Daniel Schreiber³; Pin Lu⁴; James Saal⁵; Gerald Frankel²; ¹University of Virginia; ²The Ohio State University; ³Pacific Northwest National Laboratory; ⁴Questek Innovations LLC; ⁵Citrine Informatics

2:25 PM

Tracer Diffusion in Single Crystalline CoCrFeNi and CoCrFeMnNiHigh-entropy Alloys: Kinetic Hints towards a Low-temperature PhaseInstability of the Solid-

MOBILE-FRIENDL

NIENIS

Π

9

solution?: Daniel Gaertner¹; Josua Kottke¹; Yury Chumlyakov¹; Fabian Hergemöller¹; Gerhard Wilde¹; Sergiy Divinski¹; ¹Institute of Materials Physics, University of Münster

2:45 PM

Electron and Phonon Thermal Conductivity in High Entropy Carbides with Variable **Carbon Content**: *Patrick Hopkins*¹; Christina Rost²; Trent Borman³; Mohammad Hossain³; Mina Lim⁴; Kathleen Quiambao-Tomko¹; John Tomko¹; Donald Brenner⁴; Jon-Paul Maria³; ¹University of Virginia; ²James Madison University; ³Pennsylvania State University; ⁴North Carolina State University

3:05 PM

Hyperbaric Laser Chemical Vapor Deposition of High-strength Aluminium-Silicon Carbide Nanocomposite Fibers: James Maxwell¹; Avinash Baji¹; Ben Mahler¹; ¹La Trobe University, EMC² Centre, Engineering Dept.

ADVANCED MATERIALS

High Entropy Alloys IX: Structures and Modeling - Structures and Characterization IV

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center



THURSDAY PM

Thursday PM March 18, 2021

Session Chairs: Eun Park, Seoul National University; Stefano Curtarolo, Duke University

2:00 PM Invited

Rational Use of Entropy Unavoidability in High-entropy Ceramics: Stefano *Curtarolo*¹; ¹Duke University

2:20 PM

Examination of the Bulk Metal-oxide Layer Interface of a Cr-Nb-Ta-V-W High Entropy Alloy at 700 and 800oC: Rebecca Romero¹; S.K. Varma¹; Nanthakishore Makeswaran¹; Ravisankar Naraparaju¹; C.V. Ramana¹; ¹The University of Texas at El Paso

2:40 PM

Ex-situ and In-situ Characterization of Early Stage Oxidation Mechanism of High Entropy Alloys: *Bharat Gwalani*¹; Sten Lambeets¹; Matthew Olszta¹; Daniel Perea¹; Arun Devaraj¹; ¹Pacific Northwest National Laboratory

3:00 PM

On Sluggish Diffusion in Random, Equimolar FCC Alloys: *Murray Daw*¹; Michael Chandross²; ¹Clemson University; ²Sandia National Laboratories

ADVANCED MATERIALS

Materials for High Temperature Applications: Next Generation Superalloys and Beyond — Superalloys and Beyond: Oxidation and Mechanical Behavior II



Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Thursday PM March 18, 2021

2:00 PM Invited Understanding the Oxidation Mechanisms of Complex Concentrated Refractory**based Alloys**: *Todd Butler*¹; Tinuade Daboiku¹; Joshua Gild¹; Oleg Senkov¹; ¹Wright Patterson Air Force Base

2:30 PM Invited Effect of Al Addition on the Oxidation Behavior of a Mo-Si-B Alloy: John Perepezko¹; Longfei Lu¹; ¹University of Wisconsin-Madison

3:00 PM

Oxidation Behavior of Nb-Si Based Ultrahigh Temperature Alloy at 600-1350: *Xiping Guo*¹; Xiaoyu Luo¹; Yanqiang Qiao¹; Ping Guan¹; ¹Northwestern Polytechnical University

3:20 PM

Oxidation of TiAl Alloys GE 4822 and TNM-B1 between 600°C and 900°C and



Impact on Mechanical Properties: *Mathias Galetz*¹; Lukas Mengis¹; Anke Ulrich¹; ¹DECHEMA-Forschungsinstitut

3:40 PM

On the High-temperature Air Oxidation Behavior of Ti3Al0.6Ga0.4C2 MAX Phase Solid-solution in the 1000 to 1300 °C Temperature Range: Tarek Elmeligy¹; Enrica Epifano²; Maxim Sokol¹; Michel Barsoum¹; ¹Drexel University, Department of Materials Science & Engineering, Philadelphia, PA, USA; ²Laboratoire d'Etudes des Microstructures, CNRS-ONERA, Boite Postale 72, 92322 Châtillon Cedex, France

ELECTRONIC MATERIALS

Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XX — Phase Stability of Energy Materials

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Alloy Phases Committee**

Program Organizers: Hiroshi Nishikawa, Osaka University; Shih-kang Lin, National Cheng Kung University; Chao-Hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jaeho Lee, Hongik University; Zhi-Quan Liu, Shenzhen Institutes of Advanced Technology; Ming-Tzer Lin, National Chung Hsing University; Dajian Li, Karlsruhe Institute of Technology; Yu Zhong, Worcester Polytechnic Institute; Yee-wen Yen, National Taiwan University of Science and Technology; A.S.Md Abdul Haseeb, University of Malaya; Ligang Zhang, Central South University; Sehoon Yoo, KITECH; Vesa Vuorinen, Aalto University; Yu-chen Liu, National Cheng Kung University

Thursday PM March 18, 2021



Session Chairs: Yu-chen Liu, National Cheng Kung University; Zhi-Quan Liu, Shenzhen Institutes of Advanced Technology

2:00 PM Invited Towards Predictive Solid-state Synthesis: Understanding Phase Evolution during the Formation of YBCO: Christopher Bartel¹; ¹University of California, Berkeley

2:30 PM

Machine Learning for Perovskite Phase Stability: Dane Morgan¹; Wei Li²; Ryan Jacobs¹; ¹University of Wisconsin-Madison; ²Google

2:50 PM

Vertically Stacked 2H-1T Dual-phase TMD Microstructures during Lithium Intercalation: A First Principles Study: Shayani Parida¹; Avanish Mishra¹; Jie Chen¹; Jin Wang¹; Arthur Dobley²; Barry Carter³; Avinash Dongare¹; ¹University Of Connecticut; ²EaglePicher Technologies LLC; ³Sandia National Laboratories

3:10 PM

Study on the Phase Diagrams of Bi-Te-RE (Yb, La, Ce, Nd, Sm, Tb, Er) Systems: Ligang Zhang¹; Mingyue Tan¹; Cun Mao¹; Libin Liu¹; ¹Central South University

3:30 PM

The Significance of Transport Electronic Entropy in VO_{2: Jonathan Paras}¹; Antoine Allanore¹; ¹Massachusetts Institute of Technology

3:50 PM

Electric Current Effect on the High-strain-rate Deformation of AA7075-T6 Alalloy: Yu-Ching Chen¹; Kuan-hsueh Lin¹; Yu-Chen Liu¹; Tong Chen¹; Ting-Ju Chen¹;





PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — General Topic II

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Phase Transformations Committee**

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno

; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Thursday PM March 18, 2021

Session Chair: Rongpei Shi, Lawrence Livermore National Laboratory

2:00 PM

MicrostructuralEvolutionandDeformationBehaviorduringUniaxialCompression of Al-Si Alloys: *Tingkun Liu*¹; Matthew Olszta¹; Bharat Gwalani¹; Changyong Park²; Arun Devaraj¹; ¹Pacific Northwest National Laboratory; ²Argonne National Laboratory

2:20 PM

Suppression of Samson Phase Formation in Al-Mg Alloys by Boron Addition: *Ramasis Goswami*¹; ¹Naval Research Laboratory





THURSDAY PM

2:40 PM

Transformations in Amorphous Environments near "Critical" Temperatures: *Deep Choudhuri*¹; ¹New Mexico Institute of Mining and Technology

3:00 PM

Crystallographic Transitions in Compositionally Complex Alloy Thin Films: *Daniel Goodelman*¹; Andrea Hodge¹; ¹University of Southern California

3:20 PM

Porous Graphite Fabricated by Liquid Metal Dealloying of Silicon Carbide: *Gina Greenidge*¹; Jonah Erlebacher¹; ¹Johns Hopkins University

3:40 PM

Analysis of Dendrite Fragmentation from Microgravity Solidification Experiments: *Zachary Thompson*¹; Tiberiu Stan¹; Peter Voorhees¹; Nathalie Mangelinck-Nol²; Henri Nguyen-Thi²; ¹Northwestern University; ²Aix Marseille Univ, Université de Toulon, CNRS, IM2NP, Marseille, France

NUCLEAR MATERIALS

Thermal Property Characterization, Modeling, and Theory in Extreme Environments — Structure - Thermal Property Relationships

Sponsored by: TMS Structural Materials Division, TMS: Nuclear Materials Committee

Program Organizers: Janelle Wharry, Purdue University; Mukesh Bachhav, Idaho National Laboratory; Marat Khafizov, Ohio State University; Eric Lass, University

of Tennessee-Knoxville; Vikas Tomar, Purdue University; Tiankai Yao, Idaho National Laboratory; Cody Dennett, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Thursday PM March 18, 2021

Session Chairs: Marat Khafizov, Ohio State University; Tiankai Yao, Idaho National Laboratory

2:00 PM

Mesoscale Modeling of the Effective Thermal Conductivity of a UO2-Mo Composite Nuclear Fuel: *Karim Ahmed*¹; Fergany Badry¹; ¹Texas A&M University

2:20 PM

Thermal and Mechanical Properties of Hafnon (HfSiO4), Theory and Experiments: Zhidong Ding¹; Mackenzie Ridley¹; Jeroen Deijkers¹; Naiming Liu¹; Md. Shafkat Hoque¹; John Gaskins¹; Mona Zebarjadi¹; Patrick Hopkins¹; Haydn Wadley¹; Elizabeth Opila¹; *Keivan Esfarjani*¹; ¹University of Virginia

2:40 PM Invited

First-principles Modeling of High Temperature Irradiation Resistant Thermocouple (HTIR-TC) Performance and Oxidation: Lan Li¹; *Ember Sikorski*¹; Richard Skifton²; Brian Jaques¹; ¹Boise State University; ²Idaho National Laboratory

3:10 PM

Multiphysics Mesoscale Modeling of Ablative Thermal Protection Systems: Marina Sessim¹; Linuyan Shi¹; Simon Phillpot¹; Michael Tonks¹; ¹University of Florida

3:30 PM

An Experimentally Validated Mesoscale Model for the Effective Thermal

TMS

Conductivity of U-Zr Fuels: *Karim Ahmed*¹; Fergany Badry¹; Sean McDeavitt¹; ¹Texas



SPECIAL TOPICS

2021 Technical Division Student Poster Contest — FMD 20201 Technical Division Undergraduate Student Poster Contest

Monday PM March 15, 2021

5:30-6:30 PM

Batteries Made with Calcium Could Be Better for Electric Cars or Storing Renewable Energy: *Colton Gerber*¹; Michael Woodcox¹; Manuel Smeu¹; ¹Binghamton University

SPECIAL TOPICS

2021 Technical Division Student Poster Contest — FMD 2021 Technical Division Graduate Student Poster Contest

Monday PM March 15, 2021

5:30-6:30 PM

A Flexible Aqueous Rechargeable Battery Operating Over an Extended Temperature Range: Yehong Chen¹; Ying Wang¹; ¹LSU



Degradation Characterization in Low Cobalt Lithium-ion Intercalation Cathodes: *Hernando Jesus Gonzalez Malabet*¹; Austin Gabhart¹; Megan Flannagin¹; Alex L'Antigua¹; George Nelson¹; ¹The University of Alabama in Huntsville

Using Distribution of Relaxation Times Analysis and Microstructural Characterization to Quantify the Effects of Nanoparticle Infiltrants on the Catalytic Activity of Solid Oxide Fuel Cell Anodes: *Jillian Rix*¹; Boshan Mo¹; Uday Pal¹; Srikanth Gopalan¹; Soumendra Basu¹; ¹Boston University

Utilizing Advanced Manufacturing for the Development of Advanced In-pile Sensors and Instrumentation: *Kiyo Fujimoto*¹; Thomas Holschuh¹; Lance Hone¹; Michael McMurtrey¹; Patrick Moo¹; Troy Unruh¹; Dave Estrada²; ¹Idaho National Laboratory; ²Boise State University

SPECIAL TOPICS

2021 Technical Division Student Poster Contest — MPMD 2021 Technical Division Graduate Student Poster Contest

Monday PM March 15, 2021

5:30-6:30 PM

Comparison of Laser Diffraction and Image Analysis Techniques for Particle Size-Shape Characterization in Additive Manufacturing Applications: *Jack Grubbs*¹; Kyle Tsaknopoulos¹; Christopher Massar¹; Caitlin Walde²; Aaron Birt²; Danielle Cote¹; ¹Worcester Polytechnic Institute; ²Solvus Global

Investigation of Mechanical Properties and Microstructure in Additively

Manufactured Austenitic 316L Stainless Steel: Hussam Ali¹; Nicholas Brubaker¹;

Nicolene Van Rooyen¹; Indrajit Charit¹; Michael Maughan¹; Mark Jaster²; ¹University of Idaho; ²Premier Technology

Mechanical and Microstructural Properties of FeCrAl Accident Tolerant Fuels Cladding Subjected to Flow Boiling CHF Testing: Rajnikant Umretiya¹; Donghwi Lee²; Mark Anderson²; Raul Rebak³; Jessika Rojas¹; ¹Virginia Commonwealth University; ²Universty of Wisconsin-Madison; ³GE Global Research

Micro-structure Dependent Nano-scratch Behavior in Additively Manufactured Inconel 718: Mustafa Rifat¹; Saurabh Basu¹; ¹Penn State University

SPECIAL TOPICS

2021 Technical Division Student Poster Contest — SMD 2021 Technical Division **Graduate Student Poster Contest**

Monday PM March 15, 2021

5:30-6:30 PM

Mechanical Behavior of Thermally Stable, Hierarchical Ni-Y Alloys: Shruti Sharma¹; Samuel Moehring¹; Saurabh Sharma¹; Kiran Solanki¹; Pedro Peralta¹; ¹Arizona State University

Nano-mechanical Behavior of Advanced Structural Alloys: Nandita Ghodki¹; Sundeep Mukherjee¹; ¹University of North Texas



POSTERS

Prediction and Testing of Hot Cracking Susceptibility during Local Melting in Binary and Multi Component Aluminum Alloys: Shubhra Jain¹; ¹Iowa State University

Solidification and Defects Structure Evolution in Metal Additive Manufacturing via Molecular Dynamics Simulations: Gurmeet Singh¹; Veera Sundararaghavan¹; ¹University of Michigan

SPECIAL TOPICS

2021 Technical Division Student Poster Contest — SMD 2021 Technical Division **Undergraduate Student Poster Contest**

Monday PM March 15, 2021

5:30-6:30 PM

First Principles Study of Sigma Phase Destabilization in Compositionally-complex **Stainless Steel Alloys**: *Anna Soper*¹; Savanah Diaz¹; Holly Frank¹; Jonas Kaufman²; Adam Shaw³; Kevin Laws⁴; Aurora Pribram-Jones⁵; Lori Bassman¹; ¹Harvey Mudd College; ²UC Santa Barbara; ³ California Institute of Technology; ⁴University of New South Wales; ⁵UC Merced

Utilizing CALPHAD Methods to Determine Phases in a Compositionally Complex Fe-Cr-based Alloy: Kaitlyn Paulsen¹; Alexandra Loumidis¹; Patrick Conway²; Karen Privat³; Kevin Laws³; Lori Bassman¹; ¹Harvey Mudd College; ²Jönköping University; ³University of New South Wales

ADVANCED MATERIALS

WEBSITE TMS

Advanced High Strength Steels V — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Steels Committee

Program Organizers: Ana Luiza Araujo, CBMM North America Inc.; Louis Hector, General Motors Global Technical Center; Igor Vieira, Nucor Steel; Lijia Zhao, ArcelorMittal USA; Krista Limmer, CCDC Army Research Laboratory; Jonah Klemm-Toole, Colorado School of Mines; Sebastien Allain, Institut Jean Lamour; MingXin Huang, University of Hong Kong

Monday PM March 15, 2021

5:30-6:30 PM

Effect of Rolling Conditions on Microstructure and Mechanical Properties of Medium Mn Steel: *Poornachandra Satyampet*¹; Saurabh Kundu²; Prita Pant¹; ¹IIT Bombay; ²Tata Steels

ENERGY & ENVIRONMENT

Advanced Materials for Energy Conversion and Storage VII - Poster Session

Sponsored by: TMS Functional Materials Division, TMS: Energy Conversion and Storage Committee

Program Organizers: Jung Pyung Choi, Pacific Northwest National Laboratory; Soumendra Basu, Boston University; Amit Pandey, Lockheed Martin Space; Paul



Ohodnicki, University of Pittsburgh; Kyle Brinkman, Clemson University; Partha Mukherjee, Purdue University; Surojit Gupta, University of North Dakota

Monday PM March 15, 2021

5:30-6:30 PM

Session Chairs: Soumendra Basu, Boston University; Jung Pyung Choi, Pacific Northwest National Laboratory

A First-principles Study of Silver/Lanthanum Strontium Ferrite Interfacial Adhesion: *Jiyun Park*¹; Yue Qi¹; ¹Brown University

AgCl-decorated Ag Nanowire Catalysts to Maximize the Surface Effect in the Oxygen Reduction Reaction: *Suyeon Choi*¹; Youngtae Park¹; Changsoo Lee²; Hyuck Mo Lee¹; ¹Korea Advanced Institute of Science and Technology, Korea; ²Korea Institute of Energy Research

Liquid Enhanced Ga-Sn Alloy Anode for RMBs: *Jiawei Liu*¹; Chao Song¹; Yuan Yuan¹; Dajian Li¹; Fusheng Pan¹; ¹Chongqing University

MOF-derived Carbon Nanocomposites as a Novel Cathode for Lithium Air Batteries: *Hien Pham*¹; Jong-Won Lee²; Min-Sik Park¹; ¹Kyung Hee University; ²Daegu Gyeongbuk Institute of Science & Technology

Probing Structural Changes of 2D Supercapacitor Electrode by Kelvin Probe Force Microscopy: *Kowsik Sambath Kumar*¹; Nitin Choudhary¹; Deepak Pandey¹; Yi Ding¹; Luis Hurtado¹; Hee-Suk Chung²; Laurene Tetard¹; Yeonwoong Jung¹; Jayan Thomas¹; ¹University of Central Florida; ²Analytical Research Division, Korea Basic Science Institute

Synthesis and Electrochemical Performance of Nano Spinel Lithium Manganese

Oxide (LiMn2O4) Composite with Functionalized Carbon Nanostructures (CNTs, **GNPs & Graphene) by Microwave-Assisted Chemical Coprecipitation Method:** Hanan Tariq¹; Abdul Shakoor¹; Jeffin James¹; ¹Center for Advanced Materials, Qatar University

Temperature-induced Successive Martensitic and Inter-martensitic Phase Transformations of Ni_{2.15}Mn_{0.85}Ga Heusler Alloy: Amila Madiligama¹; *Pnina Ari-Gur*; Yang Ren²; Vladimir Shavrov³; Victor Koledov³; Yanling Ge⁴; James George⁵; ¹Penn State DuBois; ²Argonne National Laboratory; ³Russian Academy of Sciences; ⁴Aalto University; ⁵Western Michigan University

MATERIALS PROCESSING

Advances in Powder and Ceramic Materials Science — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Materials Characterization Committee, TMS: Powder Materials Committee

Program Organizers: Bowen Li, Michigan Technological University; Shefford Baker, Cornell University; Huazhang Zhai, Beijing Institute of Technology; Kathy Lu, Virginia Polytechnic Institute and State University; Rajiv Soman, Eurofins EAG Materials Science LLC; Faqin Dong, Southwest University of Science and Technology; Jinhong Li, China University of Geosciences (Beijing); Ruigang Wang, The University of Alabama; Eugene Olevsky, San Diego State University

Monday PM March 15, 2021

NTENTS **OF**





POSTERS

Session Chair: Kathy Lu, Virginia Polytechnic Institute and State University

Apatite Formation Ability of Ca2MgSi2O7 Bioceramic: Fariborz Tavangarian¹; Sorour Sadeghzade²; Caleb Zolko¹; Rahmatollah Emadi²; ¹Pennsylvania State University, Harrisburg; ²Isfahan University of Technology

Biodegradability and Bioactivity of Porous Hydroxyapatite-PCL-hardystonite for Using in Bone Tissue Engineering Application: Fariborz Tavangarian¹; Sorour Sadeghzade¹; Rahmatollah Emadi²; ¹Pennsylvania State University, Harrisburg; ²Isfahan University of Technology

Synthesis of Willemite Bioceramic by Mechanochemical Procedure: Sorour Sadeghzade¹; Rahmatollah Emadi²; *Fariborz Tavangarian*¹; ¹Pennsylvania State University, Harrisburg; ²Isfahan University of Technology

ELECTRONIC MATERIALS

Alloys and Compounds for Thermoelectric and Solar Cell Applications IX — **Poster Session**



Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee

Program Organizers: Hsin-Jay Wu, National Chiao Tung University; Sinn-wen Chen, National Tsing Hua University; Franck Gascoin, Cnrs Crismat Unicaen; Philippe Jund, Montpellier University; Yoshisato Kimura, Tokyo Institute of Technology; Lan Li, Boise State University; Takao Mori, National Institute for Materials Science; Tiejun Zhu, Zhejiang University; Alexandra Zevalkink, Michigan State University; Wan-Ting Chiu, Tokyo Institute of Technology

Monday PM March 15, 2021

5:30-6:30 PM

A Synergistic Approach to Boost the Thermoelectric Performance and Reduce the Thermal Conductivity in n-type PbTe : Carrier Optimization and Phase Diagram Engineering: *Ping-Yuan Deng*¹; Kuang-Kuo Wang²; Jia-Yu Du³; Hsin-Jay Wu¹; ¹National Chiao Tung University; ²National Sun Yat-sen University; ³National Tsing Hua University

Co-P Diffusion Barrier for Lead Telluride-based Thermoelectric Joints: *Kai-Wen Cheng*¹; Hsien-Chien Hsieh¹; Albert T. Wu¹; ¹National Central University

Ni/Pb-Te and Ni/Se-Sn Interfacial Reactions and Their Related Phase Diagrams: Yohanes Hutabalian¹; Zhi-kai Hu¹; Xu-hui Chen¹; Sinn-wen Chen¹; ¹National Tsing Hua University

Ultra-low Thermal Conductivity for High-Performance GeTe-based Thermoelectric Materials: *Yi-Fen Tsai*¹; Hsin-Jay Wu¹; ¹National Chiao Tung University



MOBILE-FRIENDL

Using Neutrons to Probe the Influence of Processing on Temperature-dependent Strain in PbTe: James Male¹; Riley Hanus¹; G Snyder¹; Raphael Hermann²; ¹Northwestern University; ²Oak Ridge National Laboratory

ADVANCED MATERIALS

Bulk Metallic Glasses XVIII — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Yanfei Gao, University of Tennessee-Knoxville; Hahn Choo, University of Tennessee; Yunfeng Shi, Rensselaer Polytechnic Institute; Robert Maass, Federal Institute for Materials Research and Testing (BAM); Xie Xie, FCA US LLC; Gongyao Wang, Alcoa Technical Center

Monday PM March 15, 2021

5:30-6:30 PM

Effect of Porosity Level on the Mechanical Properties of Bicontinuous Nanoporous Metallic Glasses: *Chang Liu*¹; Paulo Branicio¹; ¹University of Southern California

Characterization of Nuclear Materials and Fuels with Advanced X-ray and

Neutron Techniques – Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Nuclear Materials Committee

Program Organizers: Xuan Zhang, Argonne National Laboratory; Jonathan Almer, Argonne National Laboratory; Maria Okuniewski, Purdue University; Joshua Kane, Idaho National Laboratory; Donald Brown, Los Alamos National Laboratory; J. Kennedy, Idaho National Laboratory; Arthur Motta, Pennsylvania State University

Monday PM March 15, 2021

5:30-6:30 PM

Characterization of Microstructure, Texture, And Residual Stress in a Neutron Irradiated CANDU Pressure Tube: Abdulla Alawadi¹; *Hamidreza Abdolvand*¹; Michael Bach²; Sterling St Lawrence²; ¹Western University; ²Canadian Nuclear Laboratories

Synchrotron Microdiffraction Study of Cracks and Indentation on UO2 Material: Kun Mo¹; *Yinbin Miao*¹; Ruqing Xu¹; Tiankai Yao²; Jie Lian³; Laura Jamison¹; Abdellatif Yacout¹; ¹Argonne National Laboratory; ²Idaho National Laboratory; ³Rensselaer Polytechnic Institute

X-ray Based Nanodiffraction to Study Strain in Materials for Nuclear Energy: *Ericmoore Jossou*¹; Mehmet Topsakal¹; Xiaojing Huang¹; Khalid Hattar²; Hanfei Yan¹; Yong Chu¹; Cheng Sun³; Lingfeng He³; Jian Gan³; Lynne Ecker¹; Simerjeet Gill¹; ¹Brookhaven National Laboratory; ²Sandia National Laboratories; ³Idaho National Laboratory



CORROSION

Coatings and Surface Engineering for Environmental Protection III — Poster Session

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Arif Mubarok, PPG; Tushar Borkar, Cleveland State University; Rajeev Gupta, North Carolina State University; Mary Lyn Lim, PPG Industries; Raul Rebak, GE Global Research; Brian Okerberg, PPG Industries

Monday PM March 15, 2021

5:30-6:30 PM

Effects of Processing Conditions on the Tribocorrosion Resistance of Zr-based Thin Film Metallic Glass Coatings: *Wenbo Wang*¹; Wenjun Cai¹; ¹Virginia Polytechnic Institute and State University

Role of Surface Mechanical Attritions Processing Conditions on the Corrosion Behavior of Aluminum 7075 Alloys: *Vikrant Beura*¹; Kiran Solanki¹; ¹Arizona State University





Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Enrique Martinez Saez, Clemson University; Vahid Attari, Texas A&M University; Jorge Munoz, University of Texas at El Paso

Monday PM March 15, 2021

5:30-6:30 PM

Session Chairs: Nana Ofori-Opoku, Canadian Nuclear Laboratories; Eva Zarkadoula, Oak Ridge National Laboratory; Jorge Munoz, University of Texas El Paso; Vahid Attari, Texas A&M University; Enrique Martinez Saez, Clemson University

Martensitic Transformation in Superlattices of Two Non-transforming Materials: Shivam Tripathi¹; Michael Titus¹; Alejandro Strachan¹; ¹Purdue University

Plutonium Phase Diagrams in the New Edition of the Plutonium Handbook: Experiments and Theory: *Aurelien Perron*¹; Patrice Turchi¹; ¹Lawrence Livermore National Laboratory

CHARACTERIZATION

Data Science and Analytics for Materials Imaging and Quantification — Poster Session

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Emine Gulsoy, Northwestern University; Charudatta Phatak, Argonne National Laboratory; Stephan Wagner-Conrad, Carl Zeiss Microscopy; Marcus Hanwell, Brookhaven National Laboratory; David Rowenhorst, Naval Research Laboratory; Tiberiu Stan, Northwestern University

Monday PM March 15, 2021

5:30-6:30 PM

High Dimensional Analysis of Abnormal Grain Growth under Dynamic Annealing Conditions: *Matthew Higgins*¹; Jiwoong Kang¹; Ning Lu¹; He Liu²; Robert Suter²; Ashwin Shahani¹; ¹University of Michigan; ²Carnegie Mellon University

Quantitative EBSD Image Analysis and Prediction via Deep Learning: *Yi Han*¹; Joey Griffiths¹; Yunhui Zhu¹; Hang Yu¹; ¹Virginia Tech

Understanding Powder Morphology and Its Effect on Flowability Through Machine Learning in Additive Manufacturing: *Srujana Rao Yarasi*¹; Andrew Kitahara¹; Anthony Rollett¹; Elizabeth Holm¹; ¹Carnegie Mellon University



MATERIALS PROCESSING

TABLE

Q

ONTENTS

Deformation Induced Microstructural Modification — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: Arun Devaraj, Pacific Northwest National Laboratory; Suveen Mathaudhu, University of California-Riverside; Kester Clarke, Colorado School of Mines; Bharat Gwalani, Pacific Northwest National Laboratory; Daniel Coughlin, Los Alamos National Laboratory

March 15, 2021 Monday PM

5:30-6:30 PM

Optimization of Continuous Casting Products and High Aluminium-Magnesium Alloys Utilization in Automotive Industry Applications: Gorkem Demir¹; ¹Asas Alüminyum Sanayi ve Ticaret A.S

Synchrotron X-ray Probing Dynamic Structural Change of Materials under Shear **Deformation by High-speed Rotational Diamond Anvil Cell**: *Tingkun Liu*¹; Bharat Gwalani¹; Changyong Park²; Stas Sinogeikin³; Arun Devaraj¹; ¹Pacific Northwest National Laboratory; ²Argonne National Laboratory; ³DAC Tools, LLC

LIGHT METALS

Magnesium Technology 2021 — Poster Session

Sponsored by: TMS Light Metals Division, TMS: Magnesium Committee

Program Organizers: Victoria Miller, University of Florida; Petra Maier, University of Applied Sciences Stralsund; J. Brian Jordon, University of Alabama; Neale Neelameggham, IND LLC

Monday PM March 15, 2021

5:30-6:30 PM

Corrosion Behaviour of Shear Extruded Magnesium Alloy: Vikrant Beura¹; Vineet Joshi²; Kiran Solanki¹; ¹Arizona State University; ²Pacific Northwest National Laboratory

Corrosion Response of Friction Stir Processed EZ33 Mg Alloy: Vasanth Shunmugasamy¹; Marwa AbdelGawad¹; Eisha Khalid¹; *Bilal Mansoor*; ¹Texas A&M University at Qatar

Effect of Annealing on Microstructure and Hardness of Mg-9Al Alloy Plates Processed by Single-pass Differential Speed Rolling: Honglin Zhang¹; ZhiGang Xu¹; Sergey Yarmolenko¹; QiuMing Wei²; Laszlo Kecskes³; Jagannathan Sankar¹; ¹North Carolina A&T State University; ²University of North Carolina at Charlotte; ³Johns Hopkins University

Eutectic Modification of Mg₂Si in Mg-Si Alloys for Faster Hydrogen Absorption **Kinetics.**: *Manjin Kim*¹; Julio Piraquive¹; Yahia Ali¹; Stuart McDonald¹; Trevor Abbott²; Kazhuhiro Nogita¹; ¹University of Queensland; ²Magontec Ltd.

In situ Study of Mg-Zn Alloy Degradation Mechanisms towards Advancing In

Vitro Testing: Max Viklund¹; Lars Wadsö¹; *Dmytro Orlov*¹; ¹Lund University

Liquid Enhanced Ga-Sn Alloy Anode for RMBs: *Jiawei Liu*¹; Chao Song¹; Yuan Yuan¹; Dajian Li¹; Fusheng Pan¹; ¹Chongqing University

Mechanical and Microstructural Behavior of Rolled AZ31B Magnesium Alloy under **Three Different Stress States**: *Luiz Carneiro*¹; Duke Culbertson¹; Qin Yu²; Yanyao Jiang¹; ¹University of Nevada, Reno; ²Lawrence Berkeley National Laboratory

Optimization of Mechanical Properties in Magnesium Zinc Alloys: Christopher Hale¹; ¹North Carolina A&T University

Preparation of Thin-walled Magnesium AZ31 Alloy Tubes Using Friction Stir **Extrusion**: Vasanth Shunmugasamy¹; Eisha Khalid¹; *Bilal Mansoor*; ¹Texas A&M University at Qatar

Role of Temperature and Pre-strain in Fatigue Strength of WE43-T5 Magnesium Alloy: Marko Knezevic¹; Saeede Ghorbanpour¹; Brandon McWilliams²; ¹University of New Hampshire; ²CCDC Army Research Laboratory

NUCLEAR MATERIALS

Mechanical Behavior of Nuclear Reactor Components — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Nanomechanical Materials Behavior Committee, TMS: Nuclear Materials Committee



Program Organizers: Clarissa Yablinsky, Los Alamos National Laboratory; Assel Aitkaliyeva, University of Florida; Eda Aydogan, Middle East Technical University; Laurent Capolungo, Los Alamos National Laboratory; Khalid Hattar, Sandia National Laboratories; Kayla Yano, Pacific Northwest National Laboratory; Caleb Massey, Oak Ridge National Laboratory

Monday PM March 15, 2021

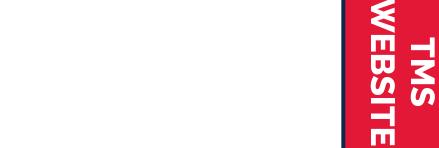
5:30-6:30 PM

Simulating the Effects of Neutron Irradiation on Zirconium Alloys: A Crystal **Plasticity Finite Element Approach**: *Omid Sedaghat*¹; Hamidreza Abdolvand¹; ¹Western University

The Thermo-mechanical Fracture of Chromium-zirconium Systems: T. Hasan¹; *Mohammed Zikry*¹; ¹North Carolina State University

MATERIALS DESIGN

Practical Tools for Integration and Analysis in Materials Engineering — Poster **Session**



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Titanium Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Adam Pilchak, US Air Force Research Laboratory; Michael Gram, Titanium Metals Corporation; William Joost; Raymundo Arroyave, Texas A&M University; Charles Ward, AFRL/RXM

Monday PM March 15, 2021

5:30-6:30 PM

An Automated Procedure for Reconstructing Deformation Twin Hierarchies in Heavily Twinned Microstructures Implemented Using MTEX: Daniel Savage¹; Rodney McCabe²; Marko Knezevic³; ¹University of New Hampshire/Los Alamos National Lab; ²Los Alamos National Laboratory; ³University of New Hampshire

Application of Prolate Spheroid Stereology to Microtexture Regions in Ti-6Al-4V: Jaylen James¹; Adam Pilchak²; Sushant Jha³; Raymundo Arroyave¹; Eric Payton²; ¹Texas A&M University; ²AFRL; ³AFRL/UDRI

Crystal Plasticity Model for Single Crystal Ni-based Superalloys: Capturing Orientation and Temperature Dependence of Flow Stress: Satyapriya Gupta¹; *Curt Bronkhorst*¹; ¹University of Wisconsin, Madison



MOBILE-FRIEND

Rare Metal Extraction & Processing — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Gisele Azimi, University of Toronto; Takanari Ouchi, The University of Tokyo; Kerstin Forsberg, KTH Royal Institute of Technology; Hojong Kim, Pennsylvania State University; Shafiq Alam, University of Saskatchewan; Alafara Baba, University of Ilorin; Neale Neelameggham, IND LLC

Monday PM March 15, 2021

5:30-6:30 PM

Extraction of Zn, Ga, Ge and In from Zinc Plant Residues: *Vivek Kashyap*¹; ¹Colorado School of Mines

ENERGY & ENVIRONMENT

Recycling and Sustainability for Emerging Technologies and Strategic Materials — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS Light Metals Division, TMS: Recycling and Environmental Technologies Committee

Program Organizers: John Howarter, Purdue University; Mingming Zhang, ArcelorMittal Global R&D; Elsa Olivetti, Massachusetts Institute of Technology; Hong Peng, University of Queensland

VEBSIT

TMS





Conductivity of AlCl3-BMIC Ionic liquid Mixtures Containing TiCl4 at Different Temperatures and Molar Ratios: Md Khalid Nahian¹; Aninda Nafis Ahmed¹; Pravin S. Shinde¹; Ramana G. Reddy¹; ¹The University of Alabama

LIGHT METALS

TMS-DGM Symposium: A Joint US-European Symposium on Linking Basic Science to Advances in Manufacturing of Lightweight Metals — Poster Session

Sponsored by: Deutsche Gesellschaft für Materialkunde e.V. (DGM): German Materials Society, TMS Materials Processing and Manufacturing Division, TMS: **Shaping and Forming Committee**

Program Organizers: William Joost; Norbert Hort, Helmholtz-Zentrum Geesthacht

Monday PM March 15, 2021

5:30-6:30 PM



The Microstructure, Morphology and Mechanical Properties of Rapidly Solidified Al-10wt%Si-0.4wt%Sc Alloy: Akankshya Sahoo¹; Abdoul Aziz Bogno¹; Hani Henein¹; ¹University of Alberta

NANOSTRUCTURED MATERIALS

100 Years and Still Cracking: A Griffith Fracture Symposium — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Nanomechanical Materials Behavior Committee

Program Organizers: Megan Cordill, Erich Schmid Institute of Materials Science; William Gerberich, University of Minnesota; David Bahr, Purdue University; Christopher Schuh, Massachusetts Institute of Technology; Daniel Kiener, Montanuniverstität Leoben; Neville Moody; Nathan Mara, University of Minnesota; Erica Lilleodden, Helmholtz-Zentrum Geesthacht

March 16, 2021 **Tuesday PM**

5:30-6:30 PM

Session Chair: Megan Cordill, Erich Schmid Institute

Crack Driving Force Expressions Using Compliance Approach in Clamped Beam Bending Geometry: Tejas Chaudhari¹; Ashwini Mishra¹; Hrushikesh Sahasrabuddhe¹; Nagamani Jaya Balila¹; ¹IIT Bombay

EAM Potential for Liquid Metal Induced Fracture: Antoine Clement¹; Thierry Auger¹;

NUCLEAR MATERIALS

Accelerated Discovery and Qualification of Nuclear Materials for Energy Applications — Poster Session

Sponsored by: TMS Structural Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee, TMS: Nuclear Materials Committee, TMS: Additive Manufacturing Committee

Program Organizers: Yongfeng Zhang, University of Wisconsin-Madison; Adrien Couet, University of Wisconsin-Madison; Michael Tonks, University of Florida; Jeffery Aguiar, Idaho National Laboratory; Andrea Jokisaari, Idaho National Laboratory; Karim Ahmed, Texas A&M University

Tuesday PM March 16, 2021

5:30-6:30 PM

Anisotropic Biaxial Creep Behavior of Textured Nb-modified Zircaloy Cladding: Mahmoud Hawary¹; K. Murty¹; ¹North Carolina State University

Defect Cluster Mobilities and Preferred Configurations in \945-zirconium: A Comparison of Two Interatomic Potentials: *Jose March-Rico*¹; Brian Wirth¹; ¹University of Tennessee Knoxville



Helium Effect on Cavity Swelling in Dual-ion Irradiated Fe and Fe-Cr Alloys: Yan-Ru Lin¹; Arunodaya Bhattacharya²; Da Chen³; Ji-Jung Kai³; Jean Henry⁴; Steven Zinkle¹; ¹University of Tennessee; ²Oak Ridge National Laboratory; ³City University of Hong Kong; ⁴CEA

Manufacturing Process Optimization of High-density LEU Targets for Mo-99 Production: *Kinam Kim*¹; Tae Won Cho¹; Sunghwan Kim¹; Kyuhong Lee¹; Yong Jin Jeong¹; ¹Korea Atomic Energy Research Institute

Mesoscale Modeling of the Effect of Interfaces on Segregation of Point Defects and Solutes and the Patterning of Extended Defects: *Karim Ahmed*¹; Abdurrahman Ozturk¹; Merve Gencturk¹; Lin Shao¹; ¹Texas A&M University

Modeling and Analysis of the Effects of the Microstructure on U-10Mo Fuel Thickness Variation during Hot Rolling: *Lei Li*¹; Vineet Joshi¹; Ayoub Soulami¹; ¹Battle Pacific Northwest National Lab

SPECIAL TOPICS

Acta Materialia Awards Poster Session — Poster Session

Program Organizer: Carolyn Hansson, University of Waterloo

Tuesday PM March 16, 2021

5:30-6:30 PM

Atom Locations of Minor Dopants and Their Role in Stabilizing the Hexagonal



Atomistic Simulation of the Formation and Fracture of Oxide Bifilms in Cast Aluminum: Jialin Liu¹; Qigui Wang²; Yue Qi¹; ¹Michigan State University; ²General Motors

Bioinspired Mechanically Active Adhesives for the Repair of Heart Bleeds: *Jingjing Wu*¹; ¹Massachusetts Institute of Technology

Concentration-dependent Atomic Mobilities in FCC CoCrFeMnNi High-entropy Alloys: Daniel Gaertner¹; ¹Institute of Materials Physics, University of Münster

Demonstrating the Potential of Accurate Absolute Cross-grain Stress and **Orientation Correlation Using Electron Backscatter Diffraction**: *Tijmen Vermeij*¹; Johan Hoefnagels¹; ¹Eindhoven University of Technology

Flash Sintering of Gadolinium-doped Ceria: Tarini Prasad Mishra¹; Rubens Roberto Ingraci Neto²; Martin Bram¹; Olivier Guillon¹; Rishi Raj³; ¹Forschungszentrum Jülich GmbH; ²Los Alamos National Laboratory; ³University of Colorado Boulder

Microstructural Optimization through Heat Treatment for Enhancing the Fracture Toughness and Fatigue Crack Growth Resistance of Selective Laser Melted Ti-6Al-4V Alloy: Punit Kumar¹; Upadrasta Ramamurty¹; ¹Nanyang Teechnological University

Orientation-designed Large Single-crystal Cu-Al-Mn Alloys by Abnormal Grain Growth and Their Enhanced Functional Properties: Sheng Xu¹; Xiao Xu¹; Toshihiro Omori¹; Ryosuke Kainuma¹; ¹Tohoku University



Titania Coated Mesoporous sSilica Particles for Sustainable Water Purification: *Ogbogu Kalu*¹; ¹University of New Brunswick

Unravelling the Role of Zinc in Magnesium Corrosion at the Nanometer Scale: *Martina Cihova*¹; ¹ETH Zurich

ADDITIVE TECHNOLOGIES

Additive Manufacturing Fatigue and Fracture V: Processing-Structure-Property Investigations and Application to Qualification — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Nik Hrabe, National Institute of Standards and Technology; John Lewandowski, Case Western Reserve University; Nima Shamsaei, Auburn University; Mohsen Seifi, ASTM International/Case Western Reserve University; Steve Daniewicz, University of Alabama

March 16, 2021 **Tuesday PM**

5:30-6:30 PM

Session Chair: Nik Hrabe, National Institute of Standards and Technology (NIST)

Effect of Laser Power, Laser Spot Size and Hatch Spacing on Mechanical and Microstructural Properties of 316L Stainless Steel Processed via Selective Laser **Melting**: *Taban Larimian*; Tushar Borkar¹; Manigandan Kannan²; Dariusz Grzesiak³; Bandar AlMangour⁴; ¹Cleveland State University; ²University of Akron; ³West



Pomeranian University of Technology; ⁴Saudi Arabia Basic Industries Corporation

Effect of Thickness on Ultrasonic Fatigue Behavior of 316L Stainless Steel Made by Powder Bed Fusion Additive Manufacturing: *Megan Trombley*¹; Qianying Shi¹; John Allison¹; ¹University of Michigan

Quantifying Surface Roughness in Additive Manufactured Ti-6AI-4V Using In-situ X-ray Imaging: *Alisha Bhatt*¹; Chu Lun Alex Leung¹; Gowtham Soundarapandivan²; Sebastian Marussi¹; Saurabh Shah¹; Robert Atwood³; Manish Tiwari¹; Peter Lee¹; ¹University College of London; ²TWI Ltd; ³Diamond Light Source Ltd

Ultrasonic Nondestructive Characterization of Hybrid Additively Manufactured 420 Stainless Steel: *Luz Sotelo*¹; Cody Pratt¹; Haitham Hadidi¹; Michael Sealy¹; Joseph Turner¹; ¹University of Nebraska Lincoln

Variation and Impact of Surface Roughness on Fatigue in Laser Powder Bed Fusion: *Rachel Evans*¹; Joy Gockel¹; Luke Sheridan¹; ¹Wright State University

ADDITIVE TECHNOLOGIES

Additive Manufacturing for Energy Applications III — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Additive Manufacturing Committee, TMS: Nuclear Materials Committee

Program Organizers: Isabella Van Rooyen, Idaho National Laboratory; Indrajit Charit, University of Idaho; Subhashish Meher, Idaho National Laboratory; Michael Kirka, Oak Ridge National Laboratory; Kumar Sridharan, University of



POSTERS

Wisconsin-Madison; Xiaoyuan Lou, Auburn University

Tuesday PM March 16, 2021

5:30-6:30 PM

Session Chair: Michael Kirka, Oak Ridge National Laboratory

Additive Manufacturing of Nuclear Spacer Grids using Inconel 718 Alloy: Observed Distortion and Proposed Distortion Control Measures for Thin Walled Structures: Syed Zia Uddin¹; Jack Beuth¹; Qu He¹; ¹Carnegie Mellon University

Aid of Additive Manufacturing of 2D Materials for Miniaturization: Yingtao Wang¹; *Xian Zhang*¹; ¹Stevens Institute of Technology

Development of Additive Manufacturing Processes for Embedding Thermocouples during Directed Energy Deposition: *Matthew McCoy*¹; Kyu Cho¹; John Shelton¹; Piyush Sabharwall¹; Isabella Van Rooyen¹; ¹Northern Illinois University

Effect of Cold Rolling on the Microstructure and the Mechanical Properties of 316L Stainless Steel Parts Produced by Laser Powder Bed Fusion (LPBF): *Louis Lemarquis*¹; Pierre-François Giroux¹; Hicham Maskrot¹; Bassem Barkia¹; Olivier Hercher¹; Frédéric Bondiguel¹; Philippe Castany²; ¹Université Paris-Saclay, CEA; ²Université de Rennes, INSA Rennes

Experimental Fabrication of Porous Additive Manufactured Material: *Luis Nunez*¹; Isabella Van Rooyen²; ¹Northern Illinois University; ²Idaho National Laboratory

Numerical Study to Predict the Effect of Surface Roughness on the Thermal

and Hydraulic Performance of Additively Manufactured Heat Exchangers: Jose Gonzalez¹; Kyu Cho¹; John Shelton¹; Piyush Sabharwall¹; Isabella Van Rooyen¹;

¹Northern Illinois University

On the In-situ Formation of Nano Oxides during Laser Powder Bed Fusion as a Function of Steel Chemistry and Atmospheric Oxygen Level: Houshang Yin¹; Pu Deng¹; Miao Song²; Mallikarjun Karadge³; Xiaoyuan Lou¹; ¹Auburn University; ²University of Michigan-Ann Arbor; ³GE Research

Process-inducedHistoryEffectsontheCreepBehaviorofAdditivelyManufactured **IN718** Alloys: Saurabh Sharma¹; Kiran Solanki¹; ¹Arizona State University

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Metals: Applications of Solidification Fundamentals - Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Solidification Committee

Program Organizers: Alex Plotkowski, Oak Ridge National Laboratory; Lang Yuan, University of South Carolina; Kevin Chaput, Northrop Grumman; Mohsen Asle Zaeem, Colorado School of Mines; Wenda Tan, University of Utah; Lianyi Chen, University of Wisconsin-Madison

Tuesday PM March 16, 2021

5:30-6:30 PM

Q

NTENTS



POSTERS

MOBILE-FRIEND

Analytical Predictions and Experimental Observations of Melt Pool Geometry in Laser Powder Bed Fusion: *Kevin Graydon*¹; Nathalia Diaz Vallejo¹; Le Zhou¹; Holden Hyer¹; Brandon McWilliams²; Kyu Cho²; Yongho Sohn¹; ¹University of Central Florida; ²CCDC Army Research Laboratory

Continuity of Eutectic Microstructures Across Melt Pool Boundaries in Laser **Powder Bed Fusion**: *Jonathan Skelton*¹; James Fitz-Gerald¹; Jerrold Floro¹; ¹University of Virginia

Creating Periodic Surface Structures Using Multiple Laser Beams: Wenxuan *Zhang*¹; Wenyuan Hou¹; Craig Arnold¹; ¹Princeton University

Effect of Deoxidizer Addition on Melt Pool Oxidation of AISI 316L during SLM **Process**: Seong Gyu Chung¹; Durim Eo¹; Jung Wook Cho¹; ¹Graduate Institute of Ferrous Technology, Postech

Energy Density on Melt Pool Dynamics and Solidification Microstructures in Laser **Powder Bed Fusion Additive Manufacturing**: *Tianyu Zhang*¹; Christopher Carter¹; Lang Yuan¹; ¹University of South Carolina

In situ X-ray Observation and Quantification of Keyhole-induced Porosity during Laser Additive Manufacturing: Yuze Huang¹; Chu Lun Alex Leung¹; Samuel J. Clark¹; Siu Lun Yeung²; Yunhui Chen¹; Lorna Sinclair¹; Sebastian Marussi¹; Kamel Fezzaa³; Jeyarajan Thiyagalingam²; Peter D. Lee¹; ¹University College London; ²Science and Technology Facilities Council; ³Argonne National Laboratory

Influence of Processing Parameters and Geometry Effects on Residual Stress **Development in Laser Powder Bed Fusion Additive Manufacturing**: Anna Hayes¹; Krishna Muralidharan¹; ¹The University of Arizona

Influence of Scan Strategies on Surface Morphology in LPBF: Emil Duong¹; Lukas

Masseling¹; Ulrich Thombansen¹; Christian Knaak¹; Paul Dionne²; *Mustafa Megahed*²;

¹Fraunhofer Institute for Laser Technology ILT; ²ESI Group

Investigation into Interfacial Mixing Behavior of Blown Powder Deposited Inconel 625- Copper Alloy Bimetallic for Improvement of Bimetallic Joint Strength: *Noah Naden*¹; Judy Schneider¹; Robin Osborne²; Paul Gradl³; ¹University of Alabama in Huntsville; ²ERC Inc./ Jacobs Space Exploration Group; ³NASA/Marshall Space Flight Center

Laser Powder Bed Fusion of Metal Composites via In Situ Dealloying: *Alyssa Chuang*¹; Adam Peters¹; Ian McCue²; Jonah Erlebacher¹; ¹Johns Hopkins University; ²JHU Applied Physics Laboratory

Melt Pool Evolution in High Power Selective Laser Melting of Nickel-based Alloy: Evgenii Borisov¹; Kirill Starikov¹; Anatoly Popovich¹; *V. A. Popovich*²; ¹Peter the Great St. Petersburg Polytechnic University; ²Delft University of Technology

On Mesoscopic Surface Formation in Metal Laser Powder Bed Fusion Process: *Shanshan Zhang*¹; Subin Shrestha¹; Kevin Chou¹; ¹University of Louisville

Spatial Variation of Thermokinetics and Corresponding Grain Morphology Evolution in Laser Surface Engineered IN718: *Mangesh Pantawane*¹; Sriswaroop Dasari¹; Srinivas Mantri¹; Rajarshi Banerjee¹; Srikumar Banerjee¹; Narendra Dahotre¹; ¹University of North Texas

Understanding Solidification of Al-Alloys Processed by Laser Powder Bed Fusion Additive Manufacturing: Holden Hyer¹; Le Zhou¹; Abhishek Mehta¹; Sharon Park¹; Thinh Huynh¹; Shutao Song¹; Kyu Cho²; Brandon McWilliams²; *Yongho Sohn*¹; ¹University of Central Florida; ²CCDC Army Research Laboratory



Using Dimensionless Numbers to Describe Process Boundaries in Laser Powder Bed Fusion: *Theresa Hanemann*¹; Christoph Seyfert¹; Armin Witte¹; Peter Holfelder¹; Astrid Rota¹; Martin Heilmaier²; ¹EOS Electro Optical Systems GmbH; ²Karlsruhe Institute of Technology

WireArcAdditiveManufacturingofNano-treatedHighStrengthAluminumAlloys: Maximilian Liese¹; Maximilian Sokoluk¹; Yitian Chi¹; Xiaochun Li¹; ¹SciFacturing Lab

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Materials Design and Alloy Development III -- Super Materials and Extreme Environments — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee

Program Organizers: Behrang Poorganji, University of Waterloo; Hunter Martin, HRL Laboratories LLC; James Saal, Citrine Informatics; Orlando Rios, Oak Ridge National Laboratory; Atieh Moridi, Cornell University; Jiadong Gong, Questek Innovations LLC

Tuesday PM March 16, 2021

5:30-6:30 PM

Comprehensive Study on Creep Performance of Selective Laser Melted Inconel 718 through Post Heat Treatment and Microstructure-based Modelling: Shun Wu¹; ¹Monash University

Design and Development of Multi-Microlattice Structures for Improved



Mechanical Behavior: *Bikram Sahariah*¹; Akshay Namdeo¹; Prasenjit Khanikar¹; ¹Indian Institute of Technology Guwahati

Influence of Heat Treatments on the Dynamic Behavior of an Additively Manufactured IN718 Alloy: Saurabh Sharma¹; Kiran Solanki¹; ¹Arizona State University

Mechanical Performance of Additively Manufactured Metallic Tetrahedral Microlattice Structure: Akshay Namdeo¹; Bikram Sahariah¹; Prasenjit Khanikar¹; ¹Indian Institute of Technology Guwahati

Synchrotron Imaging of the Influence of Oxidation with Powder Age on Cracking Phenomena during Laser Powder Bed Fusion of CM247: David Rees¹; Chu Lun Alex Leung¹; Gowtham Soundarapandiyan²; Sebastian Marussi¹; Saurabh Shah¹; Robert Atwood³; Ben Saunders⁴; Gavin Baxter⁴; Peter Lee¹; ¹University College London; ²Coventry University; ³Diamond Light Source Ltd.; ⁴Rolls-Royce plc.

ADDITIVE TECHNOLOGIES

Additive Manufacturing: Solid-State Phase Transformations and Microstructural Evolution — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Phase Transformations Committee, TMS: Shaping and Forming Committee

Program Organizers: Bij-Na Kim, Carpenter Additive; Andrew Wessman, University of Arizona; Chantal Sudbrack, National Energy Technology Laboratory; POSTERS

Eric Lass, University of Tennessee-Knoxville; Katerina Christofidou, University of Sheffield; Peeyush Nandwana, Oak Ridge National Laboratory; Rajarshi Banerjee, University of North Texas; Whitney Poling, General Motors Corporation; Yousub Lee, Oak Ridge National Laboratory

Tuesday PM March 16, 2021

5:30-6:30 PM

A Comparison of the Microstructure in Blown Powder Deposition Inconel 718 for Various Heat Treatments: *Giancarlo Puerto*¹; Chris Hill²; Judy Schneider¹; ¹University of Alabama in Huntsville; ²NASA Space Flight Center

Constituent Phases and Microstructure of Cu-10Sn Alloy Produced by Laser **Powder Bed Fusion**: *Le Zhou*¹; Binghao Lu²; Holden Hyer²; Abhishek Mehta²; Sun Hong Park³; Yongho Sohn²; ¹Marquette University; ²University of Central Florida; ³POSCO Technical Research Laboratories

Effect of Hot Isostatic Pressing Conditions on Microstructure Evolution and Hardness of Laser Powder Bed Fusion Processed Alloy 718: Hamza Fagiha¹; Runbo Jiang²; Joseph Pauza²; Magnus Ahlfors³; Chad Beamer³; Anthony Rollett²; Amir Mostafaei¹; ¹Illinois Institute of Technology; ²Carnegie Mellon University; ³Quintus Technologies

In Situ Observation of Phase Evolution in Ti-6Al-4V upon Laser Processing with Synchrotron X-ray Diffraction Analysis: Seunghee Oh¹; Rachel Lim¹; Joseph Aroh¹; Joseph Pauza¹; Andrew Chuang²; Benjamin Gould²; Niranjan Parab²; Joel Bernier³; Tao Sun⁴; Robert Suter¹; Anthony Rollett¹; ¹Carnegie Mellon University; ²Argonne National Laboratory; ³Lawrence Livermore National Laboratory; ⁴University of Virginia

TMS WEBSITE

Microstructure-defect Printability in Laser Powder Deposition of Ni-based

Superalloys: *Xueqin Huang*¹; ¹Texas A&M University

Microstructure Evolution in Laser Deposited AISI 420 Stainless Steel: Effect of **Post-processing Heat Treatment**: *Madhavan Radhakrishnan*¹; Md Mehadi Hassan¹; David Otazu²; Thomas Lienert²; Osman Anderoglu¹; ¹University of New Mexico; ²Optomec Inc

Tailoring Microstructure of Selective Laser Melted TiAl-alloy with In-situ Heat Treatment via Multiple Laser Exposure: Igor Polozov¹; Artem Kantyukov¹; Anatoly Popovich¹; V. A. Popovich²; ¹Peter the Great St. Petersburg Polytechnic University; ²Delft University Of Technology

Well-aligned nanoprecipitates in Nickel alloy produced by direct metal laser sintering: Bo Yang¹; Zhongxia Shang¹; Jie Ding¹; Jack Lopez²; William Jarosinski²; Tianyi Sun¹; Yifan Zhang¹; Nicholas Richter¹; Haiyan Wang¹; Xinghang Zhang¹; ¹School of Materials Engineering, Purdue University; ²Praxair Surface Techonologies Inc.

CHARACTERIZATION

Advanced Characterization Techniques for Quantifying and Modeling **Deformation — Poster Session**

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Materials **Characterization Committee**

Program Organizers: Rodney McCabe, Los Alamos National Laboratory; Marko

Knezevic, University of New Hampshire; Irene Beyerlein, University of California-Santa Barbara; Wolfgang Pantleon, Technical University of Denmark; C. Tasan, Massachusetts Institute of Technology; Arul Kumar Mariyappan, Los Alamos National Laboratory; Olivia Underwood, Sandia National Laboratories

Tuesday PM March 16, 2021

5:30-6:30 PM

Magnetic Anisotropy and Stacking Faults in Ag/Pt/Co/Pt Multilayer Thin Films: *Yukun Liu*¹; Michael Kitcher¹; Marc De Graef¹; Vincent Sokalski¹; ¹Carnegie Mellon University

MATERIALS DESIGN

AI/Data Informatics: Applications and Uncertainty Quantification at Atomistics and Mesoscales — Poster Session I

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: **Computational Materials Science and Engineering Committee**

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Tuesday PM March 16, 2021

5:30-6:30 PM

WEBSITE TMS

CONTENTS **FABLE OF** MOBILE-FRIENDLY TECHNICAL PROGRAM

A Machine Learning Investigation of Crystallographic Parameters for Abnormal Grain Growth: Meizhong Lyu¹; Joseph Pauza¹; Ryan Cohn¹; Elizabeth Holm¹; ¹Carnegie Mellon University

A Sensitivity Analysis of Microstructure-Based Model for U-10Mo Hot Rolling and Annealing: Yucheng Fu¹; William E Frazier III¹; Kyoo Sil Choi¹; Lei Li¹; Zhijie Xu¹; Vineet V Joshi¹; Ayoub Soulami¹; ¹PNNL

Machine Learning Approach of Molecular Dynamics Simulations for Body-**Centered Cubic Zirconium**: *Vanessa Meraz*¹; Bethuel Khamala¹; Armando Garcia¹; Adrian De La Rocha¹; Jorge Munoz¹; Tess Smidt²; Wibe de Jong²; ¹The University of Texas at El Paso; ²Lawrence Berkeley National Laboratory

Microstructure-driven Parameter Calibration for Mesoscale Simulation: Theron *Rodgers*¹; Dan Bolintineanu¹; Daniel Moser¹; Reeju Pokharel²; ¹Sandia National Laboratories; ²Los Alamos National Laboratory

Mining Structure-property Linkages in Nonporous Materials Using Interpretative **Deep Learning Approach**: *Haomin Liu*¹; Niaz Abdolrahim¹; ¹University of Rochester

PHYSICAL METALLURGY

Defect and Phase Transformation Pathway Engineering for Desired Microstructures – Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee



POSTERS

Program Organizers: Yufeng Zheng, University of Nevada-Reno ; Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Timofey Frolov, Lawrence Livermore National Laboratory; Stoichko Antonov, Max-Planck-Institut für Eisenforschung GmbH; Jessica Krogstad, University of Illinois at Urbana-Champaign; Bin Li, University of Nevada, Reno

Tuesday PM March 16, 2021

5:30-6:30 PM

Anisotropic Thermal Lattice Expansion and Crystallographic Structure of Strontium Aluminide within Al-10Sr Alloy as Measured by In-situ Neutron **Diffraction**: *Klaus-Dieter Liss*¹; Stefanus Harjo²; Takuro Kawasaki²; Kazuya Aizawa²; Pingguang Xu³; ¹Guangdong Technion - Israel Institute of Technology (GTIIT); ²J-PARC Center, Japan Atomic Energy Agency; ³Materials Sciences Research Center, Japan Atomic Energy Agency

Deformation Induced Precipitation (DIP): A Cohesive Processing Strategy to Strengthen Magnesium Alloys: Suhas Eswarappa Prameela¹; Peng Yi¹; Laszlo Kecskes¹; Michael Falk¹; Timothy Weihs¹; ¹Johns Hopkins University

The Effects of Defect Structure on Transformation Properties in NiTi Alloys for Phase Change Thermal Management Applications: Asher Leff¹; Adam Wilson¹; Darin Sharar¹; ¹CCDC Army Research Laboratory

CORROSION

TMS

Environmentally Assisted Cracking: Theory and Practice — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and **Environmental Effects Committee**

Program Organizers: Bai Cui, University of Nebraska-Lincoln; Raul Rebak, GE Global Research; Srujan Rokkam, Advanced Cooling Technologies Inc; Jenifer Locke, Ohio State University

Tuesday PM March 16, 2021

5:30-6:30 PM

Session Chair: Srujan Rokkam, Advanced Cooling Technologies

Extraction of Zinc from Zinc Hypoxide in the Process of Ammonia Leaching: Linfei Zhao¹; *Hui Li*¹; Jinglong Liang¹; ¹North China University of Science and Technology

The Impact of Laser Shock Peening Parameters on the Ability to Mitigate Stress **Corrosion Cracking in Al-Mg Alloys**: *Eric Dau*¹; William Golumbfskie²; Matthew McMahon²; ¹Vision Point Systems; ²Naval Surface Warfare Center, Carderock Division

MATERIALS DESIGN

Fatigue in Materials: Fundamentals, Multiscale Characterizations and **Computational Modeling – Poster Session**

Sponsored by: TMS Structural Materials Division, TMS Materials Processing



and Manufacturing Division, TMS: Additive Manufacturing Committee, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Garrett Pataky, Clemson University; Ashley Spear, University of Utah; Antonios Kontsos, Drexel University; Brian Wisner, Ohio University; Jean-Charles Stinville, University of California-Santa Barbara

Tuesday PM March 16, 2021

5:30-6:30 PM

Micro-scale Characterization of Life-limiting Areas in Additive Manufactured **Parts**: *Connor Varney*¹; Paul Rottmann¹; ¹University of Kentucky

The Effect of Corrosion Location Relative to Local Stresses on the Fatigue Life of Geometrically-complex, Galvanically Corroded AA7075-T6: Carly Cocke¹; James Burns¹; ¹University of Virginia

PHYSICAL METALLURGY

Frontiers in Solidification Science VIII — Poster Session



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS: Phase Transformations Committee, TMS: Solidification Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Damien Tourret, IMDEA Materials; Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koc University; Tiberiu Stan, Northwestern University

Tuesday PM March 16, 2021

5:30-6:30 PM

Session Chairs: Amy Clarke, Colorado School of Mines; Ulrike Hecht, Access e.V.; Nana Ofori-Opoku, Canadian Nuclear Laboratories; Melis Serefoglu, Koç University; Tiberiu Stan, Northwestern University; Damien Tourret, IMDEA Materials

Data-assimilation for Dendritic Solidification Using Phase-field Simulation Based on Limited Observation Data: *Yuki Imai*¹; Shinji Sakane¹; Tomohiro Takaki¹; ¹Kyoto Institute of Techonology

Electronic-structure Calculations of Local Orders in Liquid Metals: *Byeongchan Lee*¹; Geun Woo Lee²; ¹Kyung Hee University; ²Korea Research Institute of Science and Standards

Multi-phase-field Lattice Boltzmann Modeling and Simulations for Semi-solid



Deformation: *Namito Yamanaka*¹; Shinji Sakane¹; Tomohiro Takaki¹; ¹Kyoto Institute of Technology

NANOSTRUCTURED MATERIALS

Heterostructured and Gradient Materials (HGM IV): Tailoring Heterogeneity for Superior Properties — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Yuntian Zhu, City University of Hong Kong; Kei Ameyama, Ritsumeikan University; Irene Beyerlein, University of California-Santa Barbara ; Yves Brechet, Grenoble Institute of Technology; Huajian Gao, Nanyang Technological University; Hyoung Seop Kim, Pohang University of Science and Technology; Ke Lu, Institute of Metal Research; Xiaolei Wu, Chinese Academy of Sciences

Tuesday PM March 16, 2021

5:30-6:30 PM

Effect of Layer Spacing and Elastic-plastic Mismatch on Fracture Toughness of Ti-TiN Multilayers: *Ashwini Mishra*¹; Hariprasad Gopalan²; Marcus Hans³; Christoph Kirchlechner⁴; Jochen Schneider³; Gerhard Dehm²; Nagamani Balila¹; ¹Indian Institute of Technology Bombay; ²Max-Planck-Institut für Eisenforschung GmbH; ³RWTH Aachen University; ⁴Karlsruhe Institute of Technology

Evolution of Diffusion Joint of Al-steel Clad Strip during Heat Treatment: *Barbora Krivská*¹; Michaela Šlapáková¹; Rostislav Králík¹; Lucia Bajtošová¹; Miroslav Cieslar¹; Mykhailo Stolbchenko²; Olexandr Grydin²; Mirko Schaper²; ¹Charles University;

Hierarchical Morphologies in Co-sputter Deposited Immiscible Alloy Thin Films: Max Powers¹; ¹University of Michigan

Origin of Enhanced Ductility in Laser Rapid Solidified Heterogeneous Hypereutectic Al-20Si Alloy: Slip Interactions between Soft Al Matrix and Hard Si Fibers?: *Huai-Hsun Lien*¹; ¹University of Michigan

Work Hardening of Gradient FeCrAl Alloy: An *In- situ* Micropillar Compression Study: *Tianyi Sun*¹; Zhongxia Shang²; Jaehun Cho²; Jie Ding²; Yifan Zhang²; Tongjun Niu²; Bo Yang²; Dongyue Xie³; Jian Wang³; Haiyan Wang²; Xinghang Zhang²; ¹Purdue University; ²Purdue University, School of Materials Engineering; ³University of Nebraska-Lincoln

MATERIALS PROCESSING

High Temperature Electrochemistry IV — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS: Nuclear Materials Committee, TMS: Hydrometallurgy and Electrometallurgy Committee

Program Organizers: Prabhat Tripathy, Batelle Energy Alliance (Idaho National Laboratory); Guy Fredrickson, Idaho National Laboratory

Tuesday PM March 16, 2021

5:30-6:30 PM



MOBILE-FRIEND

Investigation on Preparation of Fe-Al Alloys by Direct Reduction of Fe2O3-Al2O3 Powder in CaCl2-NaCl Molten Salt System: Jinrui Liu¹; *Hui Li*¹; Jinglong Liang¹; ¹North China University of Science and Technology

NUCLEAR MATERIALS

Materials and Chemistry for Molten Salt Systems — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Corrosion and Environmental Effects Committee

Program Organizers: Stephen Raiman, Texas A&M University; Kumar Sridharan, University of Wisconsin-Madison; Nathaniel Hoyt, Argonne National Laboratory; Jinsuo Zhang, Virginia Polytechnic Institute and State University; Michael Short, Massachusetts Institute of Technology; Raluca Scarlat, University of California-Berkeley

Tuesday PM March 16, 2021

5:30-6:30 PM

Session Chair: Stephen Raiman, Texas A&M University

A High-temperature Thermodynamic Reference Electrode Enclosed in an Alumina Tube: *Mingyang Zhang*¹; Jinsuo Zhang¹; ¹Virginia Tech

An Update on the Round Robin for Molten Salt Chemical and Thermal Properties

Characterization: Raluca Scarlat¹; Theodore Bessman²; Jake McMurray³; ¹University

High-temperature, Air-compatible Molten Salts, and an Associated Corrosion-

Cost-effective, Reliable Containment of High-temperature Molten Chlorides for Heat Transfer and Thermal Energy Storage: *Liangjuan Gao*¹; Elizabeth Laskowksi¹; Kenneth McGowan¹; Robert Cullen¹; Mario Caccia¹; Kenneth Sandhage¹; ¹Purdue University

Development and Demonstration of a Novel Spectroelectrochemical Cell for Molten Salts: *Dimitris Killinger*¹; Supathorn Phongikaroon¹; ¹Virginia Commonwealth University

Electron Energy Loss Spectroscopy Characterization of Molten Salt Corrosion Damage in Pure Ni and Model Ni-20Cr Binary Alloy: *Kaustubh Bawane*¹; Panayotis Manganaris¹; Yachun Wang¹; Jagadeesh Sure²; Arthur Ronne³; Xiaoyang Liu³; Phillip Halstenberg⁴; Simerjeet Gill²; Kotaro Sasaki²; Yu-chen Karen Chen-Wiegart³; Shannon Mahurin⁴; Simon Pimblott¹; James Wishart²; Lingfeng He¹; ¹Idaho National Laboratory; ²Brookhaven National Laboratory; ³Stony Brook University; ⁴Oak Ridge National Laboratory

Fast and Accurate High-dimensional Neural Network Interatomic Potentials for Lithium-based Fluoride Salts: *Stephen Lam*¹; Qing-Jie Li²; Ronald Ballinger; Charles Forsberg²; Ju Li²; ¹University of Massachusetts - Lowell; ²Massachusetts Institute of Technology

Fluoride Salt Purification Using Bifluoride Salt for Hydrogen Fluoride-generation: Ronald Laehn¹; Dakotah Martinez²; Aaron Robison¹; ¹Abilene Christian University; ²ACU NEXT Project



POSTERS

resistant Containment Strategy, for Cost-effective and Reliable Heat Transfer and Thermal Energy Storage: *Adam Caldwell*¹; Grigorios Itskos¹; Saeed Bagherzadeh¹; Mario Caccia¹; Kenneth Sandhage¹; ¹Purdue University

High-temperature, High-toughness, Corrosion-resistant Cermet Alloys (NiWC) for CSP Gen 3 Subsystem Component Design

: *Lewis Handy-Cardenas*¹; Mohamed Elbakhshwan¹; Scott Lee¹; Mark Anderson¹; Joseph Hensel²; Gabriel Santillan²; ¹University of Wisconsin-Madison; ²Powdermet

Investigating Test Parameters for Isothermal Salt Compatibility Experiments: *Cory Parker*¹; Dino Sulejmanovic¹; James Kurley¹; Stephen Raiman¹; Bruce Pint¹; ¹Oak Ridge National Laboratory

Performance of Corrosion Resistant Claddings on 316H Stainless Steel in Molten Fluoride Salt: *Matthew Weinstein*¹; Will Doniger¹; Cody Falconer¹; Chuan Zhang²; Cem Topbasi³; Kumar Sridharan¹; Adrien Couet¹; ¹University Of Wisconsin Madison; ²Computherm, LLC; ³Electric Power Research Institute

Prediction of Actinide Salt Compounds Using Density-Functional Theory and the Universal Structure Predictor: Evolutionary Xtallography (USPEX) Algorithm: *Matthew Christian*¹; Theodore Besmann¹; ¹University of South Carolina

Purification of Molten NaCl-CaCl2 Using Anhydrous HCl: *D. Hamilton*¹; ¹University of Utah

Relevance and Methods of Fluoroacidity Quantification: *Haley Williams*¹; Nicholas Winner¹; Raluca O. Scarlat¹; ¹University of California - Berkeley

Short-and Medium-range Structure of Molten Fluorides with Cr Solutes: *Nicholas Winner*¹; Haley Williams¹; Raluca Scarlat¹; Mark Asta¹; ¹University of California Berkeley

Testing Setup to Analyze Particulates in 316 Stainless Steel Molten Salt Systems:

*Reuben Howe*¹; Josh Dowell¹; Timothy Head¹; Timothy Kennedy¹; ¹ACU NEXT Lab

Yellowjacket: A New MOOSE-based Corrosion Modelling Application for Molten Salt Reactors: Parikshit Bajpai¹; Chaitanya Bhave²; Max Poschmann¹; David Andrs³; Michael Tonks²; Markus Piro¹; ¹Ontario Tech University; ²University of Florida; ³Idaho National Laboratory

MATERIALS PROCESSING

Materials Engineering -- From Ideas to Practice: An EPD Symposium in Honor of Jiann-Yang Hwang — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS: Materials Characterization Committee, TMS: Pyrometallurgy Committee

Program Organizers: Bowen Li, Michigan Technological University; Baojun Zhao, University of Queensland; Jian Li, CanmetMATERIALS; Sergio Monteiro, Instituto Militar de Engenharia; Zhiwei Peng, Central South University; Dean Gregurek, RHI Magnesita; Tao Jiang, Central South University; Yong Shi, Futianbao Environment Technologies; Cuiping Huang, FuTianBao Environment Protection Technology Company Ltd.; Shadia Ikhmayies

Tuesday PM March 16, 2021

5:30-6:30 PM

Session Chairs: Zack Li, XL Technologies, Inc; Zhiwei Peng, Central South University



Ballistic Evaluation of the Multilayer Armor System Reinforced by Guaruman **Fiber**: Raphael Reis¹; Larissa Nunes¹; *Sergio Monteiro*; Lucio Nascimento¹; ¹Military Institute of Engineering

Determination of the Elasticity Modulus of a PC/rGO Nanocomposite via Impulse **Excitation Technique - Sonelastic:** Anderson Oliveira da Silva¹; Ricardo Weber¹; Sergio Monteiro; Karollyne Monsores¹; ¹Military Institute of Engineering

Evaluation of Ballistic Behavior by Residual Velocity of Epoxy Composite **Reinforced with Sisal Fabric after UV Radiation Exposure**: *Michelle Oliveira*¹; Lucio Nascimento¹; Sergio Monteiro¹; ¹Instituto Militar de Engenharia

Influence of Surface Treatment on Physical and Chemical Behavior of **Politetrafluoroethylene**: Karollyne Monsores¹; Géssica Nicolau¹; Anderson Oliveira¹; Suzane Oliveira¹; Ricardo Weber¹; *Sergio Monteiro*; ¹Instituto Militar de Engenharia

Influence of Weathering on the Mechanical Performance of an Aramid Fabric: Anderson Oliveira da Silva¹; Ricardo Weber¹; Rodrigo Nascimento¹; Sergio Monteiro; ¹Military Institute of Engineering

Physical and Morphological Analysis of Concrete Produced with Expanded Clay: Luana Demosthenes¹; Julio Jorge Braga de Carvalho Nunes; Lisley Madeira Coelho¹; Sergio Neves Monteiro¹; Ana Maria Abreu Jorge Teixeira¹; ¹Instituto Militar de Engenharia

Structural Characterization of Caranan Fiber (Mauritiella Aramata): Andressa Souza¹; Raí Junio¹; *Lucas Neuba*¹; Raphael Reis¹; Luana Demosthenes¹; Sérgio Monteiro¹; Lúcio Nascimento¹; ¹IME

The Influence of Ultraviolet (UV) Radiation on the Surface of Coconut Fiber: Géssica Nicolau¹; Ricardo Weber¹; *Sergio Monteiro*¹; Anderson Oliveira da Silva¹;

Karollyne Monsores¹; Filipe Araújo¹; ¹Instituto Militar de Engenharia

Thermal Behavior of Epoxy Matrix Composite Reinforced with Caranan Fibers: Andressa Souza¹; Raí Junio¹; Lucas Neuba²; Fernanda da Luz²; *Sergio Monteiro*¹; Lúcio Nascimento²; ¹Instituto Militar de Engenharia; ²Instituto Militar de Engenharia

WeibullAnalysis of the Mechanical Properties of the Epoxy Composite Reinforced with Guaruman Fibers: Raphael Reis¹; Larissa Nunes¹; Sergio Monteiro; Lucio Nascimento¹; ¹Military Institute of Engineering

ADDITIVE TECHNOLOGIES

Additive Manufacturing of Functional, Energy, and Magnetic Materials — **Poster Session**

Sponsored by: TMS Functional Materials Division, TMS: Additive Manufacturing Committee, TMS: Magnetic Materials Committee

Program Organizers: Markus Chmielus, University of Pittsburgh; Sneha Prabha Narra, Worcester Polytechnic Institute; Mohammad Elahinia, University of Toledo; Reginald Hamilton, Pennsylvania State University; Iver Anderson, Iowa State University Ames Laboratory

March 17, 2021 Wednesday PM

5:30-6:30 PM



ZTEZIS

Π

Q

POSTERS

Additive Manufacturing of Soft Magnets for Electrical Machines—Prospects and Challenges: *Tej Lamichhane*¹; Latha Sethuraman²; Adrian Dalagan¹; Haobo Wang¹; Jonathan Keller²; M. Parans Paranthaman¹; ¹Oak Ridge National Laboratory; ²National Renewable Energy Laboratory

Effect of Processing Parameters on Thermal Cyclic Stability of Nitinol Alloys Manufactured by Selective Laser Melting: *Jianing Zhu*¹; Evgenii Borisov²; Johan Bijleveld¹; Eduard Farber²; Marcel Hermans¹; Vera Popovich¹; ¹Delft University of Technology; ²Peter the Great Saint-Petersburg Polytechnic University

Modeling of Selective Laser Melting of NiTi Shape Memory Alloy: Laser Single Track and Melt Pool Dimension Prediction: Hossein Abedi¹; Reza Javanbakht¹; Mohammadreza Nematollahi¹; Keyvan Safaei¹; Ala Qattawi¹; Mohammad Elahinia¹; ¹The University of Toledo

ADVANCED MATERIALS

Advanced Functional and Structural Thin Films and Coatings — Poster Session

Sponsored by: TMS Functional Materials Division, TMS: Thin Films and Interfaces Committee

Program Organizers: Adele Carrado, IPCMS - CNRS; Ramana Chintalapalle, University of Texas at El Paso; Gerald Ferblantier, Icube Laboratory - Strasbourg University; Nancy Michael, University of Texas at Arlington; Karine Mougin, Is2m Cnrs; Heinz Palkowski, Clausthal University of Technology; Nuggehalli Ravindra, New Jersey Institute of Technology; Vikas Tomar, Purdue University

March 17, 2021 Wednesday PM

TMS

5:30-6:30 PM

A Study on PMMA-copolymers Grafted onto Ti Using Advanced Chemistry Approach: *Flavien Mouillard*; Patrick Masson¹; Genevieve Pourroy¹; Adele Carrado¹; ¹IPCMS - CNRS

Atomic Layer Deposition & Atomic Layer Etching – An Overview of Selective **Processes**: Oktay Gokce¹; Nuggehalli Ravindra¹; *Samiha Hossain*¹; ¹New Jersey Institute of Technology

Calcium-phosphate Plasma Electrolytic Oxidation (PEO) Coatings on AZ31 Mg Alloy: Effects of Different Tricalcium Phosphate (TCP) Concentrations: Navid *Attarzadeh*¹; Amir Hossein Kazemi²; Maryam Molaei²; Arash Fattah-alhosseini²; ¹University of Texas at El Paso; ²Bu-Ali Sina University

Studying Effects of Frequency on ZrTiO₄/ZrO₂ Nanocomposite Coatings on Ti-6Al-4V Alloys Produced by Plasma Electrolytic oxidation (PEO) Process: Navid *Attarzadeh*¹; Elham Nikoomanzari²; Kazem Babaei²; Arash Fattah-alhosseini²; ¹University of Texas at El Paso; ²Bu-Ali Sina University

Temperature Dependence of Energy Gap in Semiconductors – Influence on Solar **Cell Performance**: Leqi Lin¹; Rayan Daroowalla²; *Ritvik Rangaraju*³; Nuggehalli Ravindra¹; ¹New Jersey Institute of Technology; ²University of Maryland; ³West Windsor-Plainsboro High School South

Advances in Surface Engineering III – Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Surface Engineering Committee

Program Organizers: Tushar Borkar, Cleveland State University; Arif Mubarok, PPG; Rajeev Gupta, North Carolina State University; Sandip Harimkar, Oklahoma State University; Bharat Jasthi, South Dakota School of Mines & Tech

Wednesday PM March 17, 2021

5:30-6:30 PM

Damage Tolerance of TiC-laden Tribaloy T400 Suspension-powder Plasmasprayed Composite Biocompatible Coating: Moumita Mistri¹; Shrikant Joshi²; Kantesh Balani¹; Kamal Kar¹; ¹Indian Institute of Technology Kanpur; ²University West

MATERIALS DESIGN

AI/Data Informatics: Applications and Uncertainty Quantification at Atomistics and Mesoscales — Poster Session II



Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Kamal Choudhary, National Institute of Standards and Technology; Garvit Agarwal, Argonne National Laboratory; Wei Chen, Illinois Institute of Technology; Mitchell Wood, Sandia National Laboratories; Vahid Attari, Texas A&M University; Oliver Johnson, Brigham Young University; Richard Hennig, University of Florida

Wednesday PM March 17, 2021

5:30-6:30 PM

Multi-fidelity Machine-learning with Uncertainty Quantification and Bayesian Optimization for Materials Design: Application to Random Alloys: Julien Tranchida¹; *Anh Tran*; Timothy Wildey¹; Aidan Thompson¹; ¹Sandia National Laboratories

Parsimonious Neural Networks Learn Classical Mechanics and an Accurate Time Integrator: Saaketh Desai¹; Alejandro Strachan¹; ¹Purdue University

Quantifying RAMPAGE Interatomic Potentials for Metal Alloys: *Elan Weiss*¹; Arun Hegde²; Cosmin Safta²; Habib Najm²; David Riegner¹; Logan Ward¹; Wolfgang Windl¹; ¹The Ohio State University; ²Sandia National Laboratories

Solving Stochastic Inverse Problems for Structure-Property Linkages Using Data-Consistent Inversion: Anh Tran¹; Tim Wildey¹; ¹Sandia National Laboratories

Use of Atomistic Based Informatics to Model Ionic Bombardment to Synthesize

Boron Carbides: *Kwabena Asante Boahen*¹; Nirmal Baishnab²; Paul Rulis³; Michelle Paquette³; Ridwan Sakidja¹; ¹Missouri State University; ²University of Missouri, Columbia; ³University of Missouri, Kansas City

MATERIALS DESIGN

AI/Data informatics: Design of Structural Materials — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Mechanical Behavior of Materials Committee, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee

Program Organizers: Jennifer Carter, Case Western Reserve University; Amit Verma, Carnegie Mellon University; Natasha Vermaak, Lehigh University; Jonathan Zimmerman, Sandia National Laboratories; Darren Pagan, Pennsylvania State University; Chris Haines, Ccdc Army Research Laboratory; Judith Brown, Sandia National Laboratories

Wednesday PM March 17, 2021

5:30-6:30 PM

Discovery of Optimized -phase Free Ti-based Alloys Using CALPHAD and Artificial Intelligence Approach: George Dulikravich¹; *Rajesh Jha*; ¹Florida International University

Evaluating Uncertainty in Clustering of Nanoindentation Mapping Data: Bernard

Becker¹; *Eric Hintsala*¹; Benjamin Stadnick¹; Douglas Stauffer¹; Ude Hangen¹; ¹Bruker

Nano Surfaces Division

Fast and High-throughput Synthesis of Film and Bulk High-entropy Alloys: Yu *Zou*¹; ¹University of Toronto

High-throughput Calculation to Predict the Eutectic Point in Quaternary System: Jun Lu¹; Yu Zhong¹; ¹Worcester Polytechnic Institute

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering — Poster **Session**

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS: Phase Transformations **Committee, TMS: Solidification Committee**

Program Organizers: Mohsen Asle Zaeem, Colorado School of Mines; Mikhail Mendelev, KBR; Bryan Wong, University of California, Riverside; Ebrahim Asadi, University of Memphis; Garritt Tucker, Colorado School of Mines; Charudatta Phatak, Argonne National Laboratory; Bryce Meredig, Citrine Informatics

Wednesday PM March 17, 2021

5:30-6:30 PM

Session Chair: Mohsen Asle Zaeem, Colorado School of Mines



Model and Improved Dynamic Programming Algorithm for Optimization of **Unplanned Slab Allocation in the Steel Plant**: *Yongzhou Wang*¹; Zhong Zheng¹; Cheng Wang¹; Xiaoqiang Gao¹; ¹Chongqing University

BIOMATERIALS

Biological Materials Science – Poster Session

Sponsored by: TMS Functional Materials Division, TMS Structural Materials **Division, TMS: Biomaterials Committee**

Program Organizers: David Restrepo, University of Texas at San Antonio; Steven Naleway, University of Utah; Jing Du, Pennsylvania State University; Ning Zhang, University of Alabama

Wednesday PM March 17, 2021

5:30-6:30 PM

Session Chairs: David Restrepo, The University of Texas at San Antonio; Jing Du, Penn State University

A Novel Cardiac Patch for Treating Myocardial Infarction: Juan Sebastian Rincon *Tabares*¹; Juan Camilo Velasquez¹; Hayden Bilbo¹; Hai-Chao Han¹; David Restrepo¹; ¹The University of Texas at San Antonio

Bone-Mimetic B-TNTZ Alloy for Osteointegration and Antibacterial Property: A



Hospital, Taiwan



Strain Field Mining of Steady-state Tearing Fields in Thin Film, Heterogeneous Fiber Networks: Sarah Paluskiewicz¹; Christopher Muhlstein¹; ¹Georgia Institute of Technology

NUCLEAR MATERIALS

Ceramic Materials for Nuclear Energy Research and Applications – Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS Structural Materials Division, TMS Light Metals Division, TMS: Advanced Characterization, Testing, and Simulation Committee, TMS: Energy Committee, TMS: Nuclear Materials Committee

Program Organizers: Xian-Ming Bai, Virginia Polytechnic Institute and State University; Yongfeng Zhang, University of Wisconsin-Madison; Larry Aagesen, Idaho National Laboratory; Vincenzo Rondinella, Jrc-Ec

Wednesday PM March 17, 2021

5:30-6:30 PM

Session Chair: Yongfeng Zhang, University of Wisconsin - Madison

A Model of Grain Boundary Energy Anisotropy in Uranium Dioxide Nuclear Fuel:

Dallin Fisher; Evan Hansen¹; Yongfeng Zhang²; Sean Masengale²; Axel Seoane³; Timothy Harbison¹; ¹Brighan Young University-Idaho; ²University of Wisconsin-Madison; ³Virginia Tech

Development of Hydrothermal Corrosion Barrier Coatings for High-density Nuclear Fuels: John Lacy¹; Hwasung Yeom¹; Kyle Quillin¹; Kathryn Metzger²; Edward Lahoda²; Kumar Sridharan¹; ¹University of Wisconsin - Madison; ²Westinghouse Electric Company

Hydrothermal Corrosion Study of Additive Manufactured SiC Fibers: Arunkumar Seshadri¹; Akshay Dave¹; Bren Phillips¹; Koroush Shirvan¹; Shay Harrison²; Joseph Pegna²; ¹Massachusetts Institute of Technology; ²Free Form Fibers

CHARACTERIZATION

Characterization of Minerals, Metals and Materials 2021 — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS: Materials **Characterization Committee**

Program Organizers: Jian Li, CanmetMATERIALS; Mingming Zhang, ArcelorMittal Global R&D; Bowen Li, Michigan Technological University; Sergio Monteiro, Instituto Militar de Engenharia; Shadia Ikhmayies; Yunus Kalay, Middle East Technical University; Jiann-Yang Hwang, Michigan Technological University; Juan Escobedo-Diaz, University of New South Wales; John Carpenter, Los Alamos National Laboratory; Andrew Brown, Army Research Laboratory; Rajiv Soman, Eurofins EAG Materials Science LLC; Alex Moser, US Naval Research Laboratory

Wednesday PM March 17, 2021

TMS

5:30-6:30 PM

Chemical Characterization of Hemp Fabric for Engineering Composites

Session Chairs: Rajiv Soman, Eurofins EAG Materials Science LLC; Yunus Kalay, Middle East Technical University

Analysis of Potential Applications of Kamafugite Rocks in Fertilizer: Rodrigo Motta¹; Edson Mattiello¹; Fabiane Ballotin¹; Patrícia Matias¹; *Gustavo Lima*; Leonardo Pedroti¹; Jéferson Martins²; Luiz Silveira²; ¹Federal University of Viçosa; ²Terra Brasil Minerals

Application of Desulphurization Residue in Cementitious Mortars: Ariana Azeredo¹; Afonso Azevedo; Markssuel Marvila¹; Lucas Reis¹; José Alexandre Linhares Júnior¹; Carlos Maurício Vieira¹; Jonas Alexandre¹; Sergio Monteiro²; ¹Universidade Estadual do Norte Fluminense Darcy Ribeiro; ²IME

Ballistic Behavior of Epoxidic Matrix Composites Reinforced with Graphene **Oxide Functionalized Curauá Fibers**: *Ulisses Costa*¹; Lucio Nascimento¹; Wendell Almeida Bezerra¹; Sergio Monteiro¹; ¹Military Institute of Engineering

Ballistic Behavior of Epoxy Matrix Composites Reinforced with Hemp Fabric Against .22 Ammunition: Matheus Ribeiro¹; ¹Military Institute of Engineering

Characterization of Epoxidic Matrix Composites Reinforced with Graphene **Oxide Functionalized Curaua Fibers**: *Ulisses Costa*¹; Lucio Nascimento¹; Wendell Almeida Bezerra¹; Sergio Monteiro¹; ¹Military Institute of Engineering

Characterization of Piassava Fiber Collected as Industrial Waste: Juliana Carvalho¹; Noan Simonassi¹; *Felipe Lopes*¹; Carlos Vieira¹; ¹UENF



POSTERS

ONTENTS

TABLE

Q

Applications: Matheus Ribeiro¹; ¹Military Institute of Engineering

Chemical, Physical and Morphological Characterization of Eco-clinker Produced From Industrial Waste: André Oliveira¹; Leonardo Pedroti¹; Guilheme Brigolini²; José Maria Franco de Carvalho¹; José Carlos Lopes Ribeiro¹; Cássia de Souza¹; Marina Altoé²; Ana Carolina Martins Pereira¹; Wellington Fernandes¹; Beatryz Cardoso Mendes¹; Caio Torres¹; Gustavo Emílio Soares de Lima¹; Márcia Maria Salgado Lopes¹; ¹Federal University of Viçosa; ²Federal University of Ouro Preto

Comparative Analysis of Mechanical Resistance and Corrosion of the Welded Region of Stainless Steel Lean Duplex 2102 and Stainless Steel Duplex 2205: Rômulo Candido¹; Niander Cerqueira¹; Victor Souza¹; Daniel Gallo¹; *Afonso Azevedo*; ¹Centro Universitário Redentor

Comparison Between Red Ceramic Parts With and Without Ornamental Stone Waste Under Weting and Drying Cycles: Mateus Moraes¹; Gustavo Xavier¹; Afonso *Azevedo*²; Jonas Alexandre¹; Markssuel Marvila¹; Sergio Monteiro³; Josinaldo Dias¹; ¹UENF; ²Fluminense Federal University; ³IME

Compressive Properties of Additively Manufactured Titanium Carbide: Heet Amin¹; Jianshen Wang¹; Daniel East²; Ali Ameri¹; Hongxu Wang¹; Evgeny Morozov¹; Juan Escobedo-Diaz¹; ¹University of New South Wales; ²CSIRO Manufaturing

Correlation between Density and Diameter Variation of Carnauba Fibers: Raí Junio¹; Lúcio Nascimento¹; Lucas Neuba¹; Andressa Souza¹; Luana Demosthenes¹; Sergio Monteiro²; ¹Military Institute of Engineering; ²Instituto Militar de Engenharia

Critical Length and Interfacial Strength of Sedge Fiber Embedded in Epoxy Matrix: Lucas Neuba¹; Andressa Souza¹; Raí Junio¹; Matheus Ribeiro¹; Raphael Reis¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

Density Weibull Analysis of tucum fiber with Different Diameters: Michelle *Oliveira*¹; Fabio Garcia Filho¹; Fernanda da Luz¹; Sergio Monteiro¹; ¹Instituto Militar

Determination of the Crystallinity Index and Morphological Aspect of Carnauba Fibers: Raí Junio¹; Lúcio Nascimento¹; Lucas Neuba¹; Andressa Souza¹; Raphael Reis¹; *Sergio Monteiro*²; ¹Military Institute of Engineering; ²Instituto Militar de Engenharia

Development of Artificial Stone with Industrial Solid Waste from Fluorescent Lamps in a Polymer Matrix: *Vitor Souza*¹; Elaine Aparecida Costa¹; Carlos Maurício Vieira¹; Sérgio Neves Monteiro²; Geovana Carla Delaqua¹; Daniele Tavares Campos³; ¹Universidade Estadual do Norte Fluminense Darcy Ribeiro; ²Instituto Militar de Engenharia; ³Instituto Federal do Espírito Santo

Dynamic Behavior of a High Hardness Ballistic Steel: Suzane Oliveira¹; Karollyne Monsores¹; Anderson Silva¹; Géssica Nicolau¹; Ricardo Weber¹; Andersan Paula¹; *Sergio Monteiro*¹; ¹IME

Ecological Mortars with Blast Slag Residue Application: José Alexandre Linhares Júnior¹; Markssuel Marvila¹; *Afonso Azevedo*; Lucas Reis¹; Ariana Azeredo¹; Carlos Maurício Vieira¹; Sergio Monteiro²; ¹Universidade Estadual do Norte Fluminense Darcy Ribeiro; ²IME

Effect of Flying Ash as an Additive or Substitute for Portland Cement on Compression Strength in Concrete Blocks (Vibro-compacted): *Hugo García-Ortiz*¹; Aislinn M. Teja-Ruiz¹; Miguel Pérez-Labra¹; Martín Reyes-Pérez¹; Edgar Cardoso-Legorreta¹; Felipe Legorreta-García¹; Francisco Barrientos-Hernández¹; Julio Cesar Juárez T.¹; ¹Universidad Autónoma del Estado de Hidalgo

Effect of the Incorporation of Bauxite and Iron Ore Tailings on the Properties of



Clay Bricks: Beatryz Mendes¹; Leonardo Pedroti¹; Bianca Bonomo¹; Anna Carolina Lucas¹; Lívia Silva¹; Márcia Lopes¹; *Gustavo Lima*¹; ¹Universidade Federal De Vicosa

Evaluation of Different Methods of Surface Treatment of Natural Açaí Fiber Added in Cementitious Composites: *Afonso Azevedo*¹; Markssuel Marvila²; Euzébio Zanelato²; Thuany Lima²; Daiane Cecchin¹; Jessica Souza³; Marcio Barbosa¹; Sergio Monteiro⁴; Higor Azevedo²; Jonas Alexandre²; Gustavo Xavier²; ¹Fluminense Federal University; ²UENF; ³UNB; ⁴IME

Evaluation of Full Bedding Concrete Blocks Prisms with Different Laying Mortar Strength: Thuany Lima¹; *Afonso Azevedo*²; Markssuel Marvila¹; Euzébio Zanelato¹; Jonas Alexandre¹; Sergio Monteiro³; ¹UENF; ²Fluminense Federal University; ³IME

Evaluation of Izod Impact Energy of Epoxy Matrix Composites Reinforced with Hemp Fabric: *Matheus Ribeiro*¹; ¹Military Institute of Engineering

Evaluation of Izod Impact Properties of the Epoxy Matrix Composite Reinforced with Curaua Fibers Functionalized with Graphen Oxide: *Ulisses Costa*¹; Lucio Nascimento¹; Wendell Almeida Bezerra¹; Sergio Monteiro¹; ¹Military Institute of Engineering

Evaluation of Mechanical Behavior in Traction of Epoxy-Caranan Composites: Andressa Souza¹; Raí Junio¹; *Lucas Neuba*¹; Michelle Oliveira¹; Sérgio Monteiro¹; Lúcio Nascimento¹; ¹IME

Evaluation of Tensile Strength and Elastic Modulus of the Epoxy Matrix Composite Reinforced with Hemp Fabric for Engineering Applications: *Matheus Ribeiro*¹; ¹Military Institute of Engineering

Evaluation of the Correlation between the Diameters of the Sedge Fibers and a Morphological Characterization: *Lucas Neuba*¹; Andressa Souza¹; Raí Junio¹; Matheurs Dibeira¹: Daphael Deis¹: Sergio Neuca¹: ¹Military Institute of Engineering

Matheus Ribeiro¹; Raphael Reis¹; Sergio Neves¹; ¹Military Institute of Engineering

_

Evaluation of the Mechanical Behavior of Epxoy Matrix-hybrid Natural Faric Composite: Accelerated Aging by UV Radiation: Clara Caminha¹; *Michelle Oliveira*¹; Lucio Nascimento¹; Sergio Monteiro¹; ¹Instituto Militar de Engenharia

Evaluation of Thermal Healing in Pervious Concrete Pavers Produced with Reactive Powders Concrete: *Wellington Fernandes*¹; Leonardo Pedroti¹; Maurício Felisberto¹; Guilherme Botelho¹; Gustavo Lima¹; Beatryz Mendes¹; Heraldo Pitanga¹; André Oliveira¹; ¹Federal University of Vicosa

Incorporation of Porcelain Residue Powder and Mineral Wastes in Epoxy Matrix for Artificial Stone Purchase: Elaine Costa¹; *Vitor Souza*¹; Rubén Rodríguez¹; Gabriela Barreto¹; Sérgio Monteiro¹; Carlos Maurício Vieira¹; ¹Universidade Estadual do Norte Fluminense

Influence of Modifier Admixture Based on Las in Cement Pastes: Ana Carolina Martins¹; Matheus Duarte¹; José Maria Carvalho¹; *André Oliveira*; Gabriel Arruda¹; Leonardo Pedroti¹; ¹Universidade Federal de Viçosa

Influence of the Ceramic Block Sorptivity on the Adherence of Rendering Mortars: Euzebio Zanelato¹; *Afonso Azevedo*²; Markssuel Marvila²; Thuany Lima³; Jonas Alexandre²; Sergio Monteiro⁴; Gustavo Xavier²; Carlos Vieira²; ¹IFF; ²UENF; ³UCAM; ⁴IME

Influence of the Granulometry of the Granite Residue on the Sorptivity of Ceramic Blocks: Euzebio Zanelato¹; *Afonso Azevedo*; Markssuel Marvila²; Thuany Lima³; Jonas Alexandre²; Pedro Rocha¹; Sergio Monteiro⁴; Carlos Vieira²; ¹IFF; ²UENF; ³UCAM; ⁴IME



Influence of the Incorporation of Granite Waste on the Weathering Resistance of Soil Pigment-based Paints: Márcia Lopes¹; Leonardo Pedroti¹; *Gustavo de Lima*¹; José Carlos Ribeiro¹; Gustavo Nalon¹; Beatryz Mendes¹; André Oliveira Júnior¹; ¹Federal University of Viçosa

Influence of the Mixing Processes of the Constituents of Incorporated Geopolymer Materials with Glass Waste: Lucas Reis¹; *Afonso Azevedo*²; Markssuel Marvila¹; Ariana Azeredo¹; José Alexandre Linhares Júnior¹; Niander Cerqueira³; Sergio Monteiro⁴; Carlos Mauricio Vieira¹; ¹UENF; ²Fluminense Federal University; ³UNIREDENTOR; ⁴IME

In-situ Investigation of Iron Ore Stock Pile during Its Stacking and Reclaiming Process: *Wen Pan*¹; Shaoguo Chen¹; Yapeng Zhang¹; Zhipeng Kang²; Dongqing Wang¹; ¹Beijing Key Lab of Green Recyclable Process for Iron & Steel Production Technology; ²Shougang Jingtang United Iron & Steel Co.,Ltd.

Life Cycle Assessment Applied to Red Ceramic Bricks Production Versus Red Ceramic Bricks Incorporated with Stone Wastes: A Comparative Study: Josinaldo Dias¹; Gustavo Xavier¹; *Afonso Azevedo*²; Jonas Alexandre¹; Carlos Mauricio Vieira¹; HenryColorado³; ¹UENF; ²Fluminense Federal University; ³Universidad de Antioquia

Mechanical Properties Evaluation of Epoxy Matrix Composites for Different Conditions of Volumetric Fraction of Sedge Fibers: *Lucas Neuba*¹; Andressa Souza¹; Raí Junio¹; Luana Demosthenes¹; Ulisses Costa¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

PCM Encapsulation for Incorporation in Construction Materials: *Gustavo Lima*¹; Matheus Oliveira¹; Luis Gustavo Nascimento¹; Evandro Martins¹; Joyce Carlo¹; Leonardo Pedroti¹; Nathália Albuini-Oliveira¹; Márcia Lopes¹; ¹Federal University of Viçosa

Physical, Chemical and Mechanical Characterization of AISI 316 Austenitic



CONTENTS

TABLE OF

Stainless Steel: Leonardo Pinheiro¹; Niander Cerqueira¹; Victor Souza¹; Daniel Gallo¹; *Afonso Azevedo*²; ¹UniREDENTOR; ²UENF

Research Progress of Aging Effects on Fiber Reinforced Polymer Composites: A Brief Review: *Michelle Oliveira*¹; Fernanda Da Luz¹; Sergio Monteiro¹; ¹Instituto Militar de Engenharia

Statistical Analysis of Izod Impact Resistance of an Epoxy Matrix Reinforced with Sedge Fibers: Lucas Neuba¹; Andressa Souza¹; Raí Junio¹; Matheus Ribeiro¹; Michelle Oliveira¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

Study of Face Shell Bedding Concrete Blocks Prisms with Different Laying Mortar Strength: Thuany Lima¹; *Afonso Azevedo*²; Markssuel Marvila¹; Euzébio Zanelato¹; Ana Luiza Paes¹; Jonas Alexandre¹; Sergio Neves Monteiro¹; ¹UENF; ²Fluminense Federal University

Study of Pathologies in Alkali Activated Materials Based on Slag: Markssuel Marvila¹; *Afonso Azevedo*; Euzébio Zanelato¹; Thuany Lima¹; Geovana Delaqua¹; Carlos Maurício Vieira¹; Leonardo Pedroti¹; Sergio Monteiro¹; ¹Universidade Estadual do Norte Fluminense Darcy Ribeiro

Study of the Feasibility of Incorporation Clay From Campos Dos Goytacazes - RJ, in Mortar Applied on Walls and Ceilings: Larissa Granato¹; Gustavo Xavier¹; Henry Colorado²; *Afonso Azevedo*³; Jonas Alexandre¹; Carlos Mauricio Vieira¹; Markssuel Marvila¹; ¹UENF; ²Universidad de Antioquia; ³Fluminense Federal University

Surface Characterization of Concentrated Jamesonite, in the Collectorless Flotation, in Acid, Neutral and Alkaline Medium: *Jazmín Terrazas Medina*¹; Martín Reyes Perez²; Elia Guadalupe Palacios Beas³; Mizraim Uriel Flores Guerrero⁴; Iván Alejandro Reyes Domínguez⁵; Aislinn Michelle Teja Ruiz¹; Miguel Pérez Labra¹; Francisco Raúl Barrientos Hernández¹; ¹ Universidad Autonoma del Estado de Hidalgo; ²Universidad Autónoma del Estado de Hidalgo; ³Instituto Politécnico Nacional; ⁴Universidad Tecnológica de Tulancingo. Área de Electromecánica Industrial; ⁵Universidad Autónoma del San Luis Potosí

Synergy between Cu and Cr on Localized Corrosion of the Low Alloy Steels: *Kewei Gao*¹; Luchun Yan¹; Xiaolu Pang¹; Zhimeng Guo¹; Yanjing Su¹; Lijie Qiao¹; ¹University of Science and Technology Beijing

Synthesis and Characterization of Iron Oxide Nanoparticles for Application in the Removal of Heavy Metals from the Aqueous Medium: *Arantza Córdova López*¹; Karen Rivera¹; Diana Serna¹; Laura García¹; Pedro Ramírez¹; Mizraim Flores¹; ¹Universidad Tecnológica de Tulancingo

Synthesis and Characterization of ZnO Nanoparticles Obtained from the Extract of Schinus Molle: Estrella Palacios¹; *Karime Cardenas*¹; Jenny Dominguez¹; Mizraim Flores¹; Laura García¹; Pedro Ramírez¹; ¹Universidad Tecnológica de Tulancingo

S/TEM Characterization of Interdendritic Phases in Ni-30Cr Weld Metal 52XL: *Cheng-Han Li*¹; Carolin Fink¹; John Lippold¹; Joerg Jinschek¹; ¹The Ohio State University

The Simpex-Lattice Method Application to Optimize the Design of Soil-Slag-Fly Ash Mixtures: Mateus Henrique Rodrigues¹; *Leonardo Pedroti*¹; Taciano Silva¹; Heraldo Pitanga¹; Klaus Henrique Rodrigues¹; Emerson Lopes¹; ¹Federal University of Viçosa

Thermal Analysis by Differential Scanning Calorimetry of Sedge Fibers and Epoxy Matrix Composites Reinforced with Sedge Fibers: *Lucas Neuba*¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

Technical, Environmental and Economic Advantages in the Use of Rubber Asphalt:



Mariah Soares¹; Niander Cerqueira¹; Felipe Almeida¹; *Afonso Azevedo*; Markssuel Marvila²; ¹Centro Universitário Redentor; ²UENF

Thermal Analysis of Sedge Fibers and Epoxy Matrix Composites Reinforced with Sedge Fibers: Lucas Neuba¹; Michelle Oliveira¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

Thermal Stability of Plain Arapaima Scales and Scales-reinforced Epoxy Matrix **Composites**: Wendell Bruno Almeida Bezerra¹; Ulisses Oliveira Costa¹; Michelle Souza Oliveira¹; Fernanda Santos da Luz¹; Luana Crystine da Cruz Demosthenes¹; Sergio Neves Monteiro¹; ¹Instituto Militar de Engenharia

Thermochemical Characterization of the Carnauba Fibers: Raí Junio¹; Lúcio Nascimento¹; Lucas Neuba¹; Andressa Souza¹; *Sergio Monteiro*²; ¹Military Institute of Engineering; ²Instituto Militar de Engenharia

Thermogravimetric Characterization of Epoxy Matrix Composite Reinforced with Hemp Fabric for Engineering Applications: Matheus Ribeiro¹; ¹Military Institute of Engineering

Use of Glass Waste as a Geopolymerization Reaction Activator for Ceramic Materials: Afonso Azevedo¹; Markssuel Marvila²; Euzébio Zanelato²; Thuany Lima²; Geovana Delaqua²; Sergio Monteiro³; Carlos Mauricio Vieira²; Leonardo Pedroti⁴; ¹Fluminense Federal University; ²UENF; ³IME; ⁴UFV

Variation of the Silica Module for Dosing Activated Alkali Mortars: Markssuel Marvila¹; Afonso Azevedo¹; Euzébio Zanelato¹; Thuany Lima¹; Sergio Monteiro²; Carlos Maurício Vieira²; Jonas Alexandre¹; Gustavo Xavier¹; ¹Universidade Estadual do Norte Fluminense Darcy Ribeiro; ²IME

Weibull Analysis of the Tensile Strength for Different Diameters of Cyperus Malaccensis Sedge Fibers: Lucas Neuba¹; Andressa Souza¹; Raí¹; Matheus Ribeiro¹; Ulisses Costa¹; Sergio Neves¹; ¹Military Institute of Engineering (IME)

Characterization of the Palm Fiber: A Natural Fiber from the Amazon: Edwillson Gonçalves de Oliveira Filho¹; Roberto Tetsuo Fujiyama¹; Jean da Silva Rodrigues²; Sergio Neves Monteiro³; Alisson Rios da Silva¹; Verônica Scarpini Candido¹; ¹Universidade Federal do Pará; ²Federal Institute of Pará; ³Military Engineering Institute

Evaluation of the Use of Lignocellulosic Fibers in Replacement of Synthetic Fiber in Polymer Hybrid Composites: Luciano Monteiro Almeida¹; Roberto Tetsuo Fujiyama¹; Sérgio Neves Monteiro²; Alisson Rios da Silva¹; Verônica Scarpini Candido¹; ¹Universidade Federal do Pará; ²Military Engineering Institute

ADDITIVE TECHNOLOGIES

Computational Techniques for Multi-Scale Modeling in Advanced Manufacturing — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS Extraction and Processing Division, TMS: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee

Program Organizers: Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, University of Alabama; Mei Li, Ford Motor Company; Alexandra Anderson, Gopher Resource; Srujan Rokkam, Advanced Cooling Technologies Inc



TMS WEBSITE

A Parametric Study of Grain Size and Its Volume Fraction Effect on Heterogeneous Materials Mechanical Properties: *Khaled Adam*¹; Tarek Belgasam¹; ¹Washington State University

Effect of Nozzle Injection Mode on Initial Transfer Behavior of Round Bloom: Pu Wang¹; liang Li¹; Datong Zhao²; Weidong Liu²; Songwei Wang²; Haiyan Tang¹; Jiaquan Zhang¹; ¹University of Science & Technology Beijing; ²Shanxi Taigang Stainless Steel Co., Ltd.

Study on the In-mold Flow Behavior Driven by a Subsurface Electromagnetic Stirring for IF Steel Slab Casting: Hong Xiao¹; Shaoxiang Li²; Pu Wang¹; Haiyan Tang¹; Jiaquan Zhang¹; ¹University of Science & Technology Beijing; ²School of Materials Science and Engineering, Tsinghua University

ADVANCED MATERIALS

High Entropy Alloys IX: Alloy Development and Properties — Poster Session

Sponsored by: TMS Functional Materials Division, TMS Structural Materials Division, TMS: Alloy Phases Committee, TMS: Mechanical Behavior of Materials Committee

Program Organizers: Peter Liaw, University of Tennessee; Michael Gao, National Energy Technology Laboratory; E-Wen Huang, National Chiao Tung University; Srivatsan Tirumalai, The University of Akron; Xie Xie, FCA US LLC; Gongyao



POSTERS

TABLE

Q

NTENTS

Wang, Alcoa Technical Center

Wednesday PM March 17, 2021

5:30-6:30 PM

Atom-by-atom Understanding of Atom Probe Tomography of HEAs: *Jiayuwen Qi*¹; Christian Oberdorfer¹; Emmanuelle Marquis²; Wolfgang Windl¹; ¹The Ohio State University; ²University of Michigan

Computation of Thermodynamics and Stability of FeNiCoCr(Mn/Pd) High **Entropy Alloys:** Competition between Equiatomic and Non-equiatomic: Tran Nguyen-Dung¹; Ying Chen¹; ¹Tohoku University

Fusion Plasma Relevant Erosion of Reduced Activation High Entropy Alloy-based **lPasma-facing Material**: *Owais Ahmed Waseem*¹; Kevin Woller¹; Faris Sweidan²; Ho Jin Ryu²; ¹Massachusetts Institute of Technology; ²Korea Advanced Institute of Science and Technology

High Throughput In Situ Micro-mechanical Testing of Multi-principal Element Alloy Thin Films to Enable Rapid Combinatorial Qualification: *Robert Quammen*¹; Paul F. Rottmann¹; ¹University of Kentucky

Thermal and Corrosion Behaviour of Laser-Deposited High Entropy Alloys: *Modupeola Dada*¹; Patricia Popoola¹; Ntombizodwa Mathe²; Sisa Pityana²; Samson Adeosun³; Olufemi Aramide¹; ¹Tshwane University of Technology; ²Council for Scientific and Industrial Research; ³University of Lagos, Akoka

TMS

ADVANCED MATERIALS

POSTERS

TABLE

P

NTENTS

Materials for High Temperature Applications: Next Generation Superalloys and Beyond — Poster Session

Sponsored by: TMS Structural Materials Division, TMS: Refractory Metals Committee

Program Organizers: Govindarajan Muralidharan, Oak Ridge National Laboratory; Martin Heilmaier, KIT Karlsruhe; Benjamin Adam, Portland State University; Mario Bochiechio, Pratt & Whitney; Katerina Christofidou, University of Sheffield; Eric Lass, University of Tennessee-Knoxville; Jeremy Rame, Safran Aircraft Engines; Pierre Sallot, Safran; Akane Suzuki, GE Research; Michael Titus, Purdue University

Wednesday PM March 17, 2021

5:30-6:30 PM

Creep Deformation Behavior of Ni - 33 Co Alloy: *Divya Sri Bandla*¹; Atul Chokshi¹; ¹Indian Institute of Science Bangalore

On the Quantitative Characterization of Weld Microstructures: *Noah Kohlhorst*¹; Govindarajan Muralidharan²; Roger Miller²; Ji-Cheng Zhao³; ¹Ohio State University; ²Oak Ridge National Laboratory (ORNL); ³University of Maryland, Department of Materials Science and Engineering

Reference-free Potential Development for Metal-rich Carbides: *Tyler McGilvry-James*¹; Bikash Timalsina¹; Nirmal Baishnab²; Puja Adhikari³; Saro San³; Andrew Duff⁴; Wai-Yim Ching³; Ridwan Sakidja¹; ¹Missouri State University; ²University of



MATERIALS PROCESSING

Materials Processing Fundamentals — Poster Session

Sponsored by: TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Process Technology and Modeling Committee

Program Organizers: Jonghyun Lee, Iowa State University; Samuel Wagstaff, Oculatus; Alexandra Anderson, Gopher Resource; Fiseha Tesfaye, Abo Akademi University; Guillaume Lambotte, Boston Metal; Antoine Allanore, Massachusetts Institute of Technology

Wednesday PM March 17, 2021

5:30-6:30 PM

Containerless Materials Processing for Materials Science on Earth and in Space: *Jonghyun Lee*¹; Sai Katamreddy¹; Yong Chan Cho²; Sooheyong Lee²; Geun Woo Lee²; ¹Iowa State University; ²Korea Research Institute of Standards and Science

Effect of Nitrogen on Weldability and the Microstructure in Laser Beam Welding of Duplex Stainless Steel: *Yunxing Xia*¹; Kenshiro Amatsu¹; Fumikazu Miyasaka¹; Hiroaki Mori¹; ¹Osaka University

Thermodynamic Examination of Quaternary Compounds in the Ag–Fe–(Ge, Sn)– Se Systems by the Solid-state EMF Method: Mykola Moroz¹; *Fiseha Tesfaye*; Pavlo



MOBILE-FRIENDL

ZTENTS

Q

and Environmental Engineering; ²Ivan Franko National University of Lviv; ³Lviv Polytechnic National University; ⁴Aalto University; ⁵Åbo Akademi University

PHYSICAL METALLURGY

Phase Transformations and Microstructural Evolution — Poster Session

Sponsored by: TMS Materials Processing and Manufacturing Division, TMS: Phase Transformations Committee

Program Organizers: Rongpei Shi, Lawrence Livermore National Laboratory; Yipeng Gao, Idaho National Laboratory; Fadi Abdeljawad, Clemson University; Bharat Gwalani, Pacific Northwest National Laboratory; Qi An, University of Nevada-Reno; Eric Lass, University of Tennessee-Knoxville; Huajing (Wilson) Song, Los Alamos National Laboratory

Wednesday PM March 17, 2021

5:30-6:30 PM

Dilatometric Analysis of Tempering Kinetics in a Cr-Mo-V Medium Carbon **Steel**: *Eliuth Barrera-Villatoro*¹; Octavio Vázquez-Gómez¹; Alexis Gallegos-Pérez¹; Héctor Vergara-Hernández¹; Edgar López-Martínez²; Pedro Garnica-González¹; ¹Tecnológico Nacional de México / I.T. Morelia; ²Universidad del Istmo

Exploring Non-conventional Microstructural Evolution in Titanium Alloys by Advanced Characterization and Machine Learning: Dian Li¹; Xing Zhang²; Yiliang Liao²; Yufeng Zheng¹; ¹University of Nevada, Reno; ²Iowa State University



POSTERS

Thermal and Mechanical Characterization of the Non-isothermal Tempering of an Experimental Medium-carbon Steel: Perla Díaz-Villaseñor¹; Octavio Vázquez-Gómez¹; Héctor Vergara-Hernández¹; Alexis Gallegos-Pérez¹; Edgar López-Martínez²; Bernardo Campillo³; ¹Tecnológico Nacional de México / I.T. Morelia; ²Universidad del Istmo; ³Universidad Nacional Autónoma de México

