

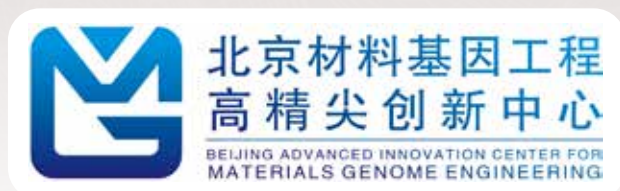


**6TH WORLD CONGRESS ON INTEGRATED  
COMPUTATIONAL MATERIALS ENGINEERING  
(ICME 2022)**

**TECHNICAL PROGRAM**

**APRIL 24–28, 2022** | Hyatt Regency Lake Tahoe  
Incline Village, Nevada, USA | [www.tms.org/ICME2022](http://www.tms.org/ICME2022)

**Sponsors:**



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**TMS**

Materials Processing &  
Manufacturing Division  
(MPMD) and the Integrated  
Computational Materials  
Engineering (ICME) Committee

**Monday Plenary**

Monday AM  
April 25, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

**8:00 AM Plenary**

An ICME Approach to Development of a Low-Cost Magnesium Sheet Component for Automotive Applications: *Bita Ghaffari*<sup>1</sup>; <sup>1</sup>Ford Motor Company

**8:40 AM Plenary**

ICME of Additively Manufactured Metals: New Computational Tools and the Central Role of Materials Data: Alexander Chadwick<sup>1</sup>; Christopher Hareland<sup>1</sup>; *Peter Voorhees*<sup>1</sup>; <sup>1</sup>Northwestern University

**9:20 AM Plenary**

DAMASK - Experiences from 10 Years ICME Software Development for Physics-based ICME: *Martin Diehl*<sup>1</sup>; Pratheek Shanthraj<sup>2</sup>; Philip Eisenlohr<sup>3</sup>; Franz Roters<sup>4</sup>; Dierk Raabe<sup>4</sup>; <sup>1</sup>KU Leuven, Max-Planck-Institut für Eisenforschung GmbH; <sup>2</sup>University of Manchester; <sup>3</sup>Michigan State University; <sup>4</sup>Max-Planck-Institut für Eisenforschung GmbH

**10:00 AM Break****Applications: Advanced Manufacturing – Additive Manufacturing I**

Monday AM  
April 25, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

**10:30 AM Invited**

Predicting As-Built Additively Manufactured Microstructures and Residual Stress Using the CAFE Model: Kirubel Teferra<sup>1</sup>; *Lukasz Kuna*<sup>2</sup>; David Rowenhorst<sup>1</sup>; <sup>1</sup>Naval Research Laboratory

**11:00 AM**

Exascale Cellular Automata for Simulating Grain Structures in Additive Manufacturing: *Sam Reeve*<sup>1</sup>; Matthew Rolchigo<sup>2</sup>; Jim Belak<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Lawrence Livermore National Laboratory

**11:20 AM**

Multiscale Modeling of Microstructure Formation in Directed Energy Deposition for Nickel-Based Superalloys: *Lang Yuan*<sup>1</sup>; Siyeong Ju<sup>2</sup>; Shenyang Huang<sup>2</sup>; Yiming Zhang<sup>2</sup>; Yang Jiao<sup>2</sup>; Chen Shen<sup>2</sup>; Hyeyun Song<sup>3</sup>; Luke Mohr<sup>3</sup>; Lee Kerwin<sup>3</sup>; Jason Parolini<sup>4</sup>; Changjie Sun<sup>2</sup>; Alex Kitt<sup>3</sup>; <sup>1</sup>University of South Carolina; <sup>2</sup>GE Research; <sup>3</sup>EWI; <sup>4</sup>GE Power

**11:40 AM**

Prediction of the Columnar-to-Equiaxed Transition During Additive Manufacturing of Concentrated Multicomponent Alloys: *Christopher Hareland*<sup>1</sup>; *Peter Voorhees*<sup>1</sup>; <sup>1</sup>Northwestern University

**12:00 PM**

Heat Source Sizing for FEA of NAB Using Wire-Fed AM: Chris Jasien<sup>1</sup>; *Charles Fisher*<sup>1</sup>; <sup>1</sup>Naval Surface Warfare Center - Carderock

**Artificial Intelligence & Machine Learning I**

Monday AM  
April 25, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

**10:30 AM Invited**

Materials Discovery via Machine Learning: Modeling Across Properties and Uncertainty Predictions: *Francesca Tavazza*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**11:00 AM**

Physics Informed Neural Networks for Modeling the Thermomechanical Properties of Additively Manufactured Metals: *Doyle Dickett*<sup>1</sup>; Sungkwang Mun<sup>1</sup>; Sara Adibi<sup>1</sup>; Matthew Priddy<sup>1</sup>; Linkan Bian<sup>1</sup>; <sup>1</sup>Mississippi State University

**11:20 AM**

AI-based High-Throughput Screening Framework for Battery Materials Design: *Alina Negoita*<sup>1</sup>; Nasim Souly<sup>1</sup>; Alina Negoita<sup>1</sup>; Prateek Agrawal<sup>1</sup>; Christian Tae<sup>1</sup>; Vedran Glavas<sup>2</sup>; Julian Wegener<sup>2</sup>; Kai Gerstner<sup>2</sup>; Alex Alekseyenko<sup>3</sup>; <sup>1</sup>VW GoA; <sup>2</sup>VW AG; <sup>3</sup>Audi oA

**11:40 AM Invited**

Advancements in EBSD Using Machine Learning: Kevin Kaufmann<sup>1</sup>; Chaoyi Zhu<sup>1</sup>; Hobson Lane<sup>1</sup>; *Kenneth Vecchio*<sup>1</sup>; <sup>1</sup>University of California, San Diego

**12:10 PM**

Prediction of Corrosion Behaviour of Additively Manufactured Nickel Based Super Alloy Using Machine Learning: *Mythreyi Venkataramana*<sup>1</sup>; Rohith Srinivaas M<sup>1</sup>; R Jayaganthan<sup>1</sup>; <sup>1</sup>IIT Madras

**ICME-Based Design Tools / Industrial Integration & Success Stories**

Monday AM  
April 25, 2022

Room: Martis Peak  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

**10:30 AM Invited**

ExtremeMAT (XMAT) – Recent Progress and Lessons Learned: Ram Devanathan<sup>1</sup>; *Laurent Capolungo*<sup>2</sup>; Jeffrey Hawk<sup>3</sup>; Ellen Cerreta<sup>2</sup>; Gabriel Ilevbare<sup>4</sup>; Matthew Kramer<sup>5</sup>; Sergei Kucheyev<sup>6</sup>; David Alman<sup>2</sup>; Edgar Lara-Curzio<sup>7</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>National Energy Technology Laboratory; <sup>4</sup>Idaho National Laboratory; <sup>5</sup>Ames National Laboratory; <sup>6</sup>Lawrence Livermore National Laboratory; <sup>7</sup>Oak Ridge National Laboratory

**11:00 AM**

A Digital Engineering Framework to Enable the Incorporation of Material Pedigree and Ddate Information into the Product Design Cycle: *Saikiran Gopalakrishnan*<sup>1</sup>; Nathan Hartman<sup>1</sup>; Michael Sangid<sup>1</sup>; <sup>1</sup>Purdue University

**11:20 AM**

Prisms-Plasticity: An Open-Source Crystal Plasticity Finite Element Software: *Mohammadreza Yaghoobi*<sup>1</sup>; Sriram Ganesan<sup>1</sup>; Aaditya Lakshmanan<sup>1</sup>; Srihari Sundar<sup>1</sup>; Duncan Greeley<sup>1</sup>; Shiva Rudraraju<sup>2</sup>; John E. Allison<sup>1</sup>; Veera Sundararaghavan<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor; <sup>2</sup>University of Michigan; University of Wisconsin-Madison

**11:40 AM**

Effects of Boundary Conditions on Microstructure-Sensitive Fatigue Crystal Plasticity Analysis: *Krzysztof Stopka*<sup>1</sup>; Mohammadreza Yaghoobi<sup>2</sup>; John Allison<sup>2</sup>; David McDowell<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>University of Michigan

12:00 PM

**A Computational Tool for Designing Protective Oxide Scale Formation:** *Youhai Wen*<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

12:20 PM

**Exploring the Vast Refractory-HEAs Composition Space: CALPHAD Database Development and Alloy Optimization:** *Aurelien Perron*<sup>1</sup>; Joel Berry<sup>1</sup>; Brandon Bocklund<sup>2</sup>; Richard Otis<sup>3</sup>; Alexander Landa<sup>2</sup>; Charles Tong<sup>1</sup>; Amit Samanta<sup>2</sup>; Hunter Henderson<sup>1</sup>; Zachary Sims<sup>1</sup>; Thomas Voisin<sup>1</sup>; Scott McCall<sup>1</sup>; Joseph McKeown<sup>1</sup>; Vincenzo Lordi<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Pennsylvania State University; <sup>3</sup>Jet Propulsion Laboratory, California Institute of Technology

## Applications: Advanced Manufacturing – Additive Manufacturing II

Monday PM  
April 25, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

1:30 PM Break

1:40 PM

**Modeling Microstructural Evolution in Laser Powder Bed Fusion with Kinetic Monte Carlo and Lattice-Boltzmann Cellular Automata Methods:** Joseph Pauza<sup>1</sup>; Guannan Tang<sup>1</sup>; Joseph Aroh<sup>1</sup>; Anthony Rollett<sup>1</sup>; *Gregory Wong*; <sup>1</sup>Carnegie Mellon University

2:00 PM

**An ICME Framework for Heat Treating Additively Manufactured Nitrogen Atomized 17-4PH Stainless Steel:** *James Zuback*<sup>1</sup>; Mark Stoudt<sup>1</sup>; Daniel Gopman<sup>1</sup>; Maureen Williams<sup>1</sup>; Carelyn Campbell<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

2:20 PM

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

## Linkage: Structure – Properties - Microstructure

Monday PM  
April 25, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

1:30 PM Invited

**ExtremeMat: Towards Microstructure and Composition Sensitive Models for the Creep Deformation of Engineering Steels:** *Laurent Capolungo*<sup>1</sup>; R. Lebensohn<sup>1</sup>; A. Kumar<sup>1</sup>; B. Beets<sup>1</sup>; A. Chakraborty<sup>1</sup>; V. Prithvirajan<sup>1</sup>; M. Gao<sup>2</sup>; M. Glazoff<sup>3</sup>; Y. Yamamoto<sup>4</sup>; M.P. Brady<sup>4</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>National Energy Technology Laboratory; <sup>3</sup>Idaho National Laboratory; <sup>4</sup>Oak Ridge National Laboratory

2:00 PM

**ICME Modeling of Fabrication of U-10%wt Mo Alloys:** *Ayoub Soulami*<sup>1</sup>; William Frazier<sup>1</sup>; Kyoo Sil Choi<sup>1</sup>; Lei Li<sup>1</sup>; Zhijie Xu<sup>1</sup>; Yucheng Fu<sup>1</sup>; Curt Lavender<sup>1</sup>; Vineet Joshi<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

2:20 PM

**Full-Field Homogenization Including Non-Local Regularization of Ductile Fracture in Heterogeneous Materials by Means of FFT:** Mira Toth<sup>1</sup>; Laurent Adam<sup>1</sup>; *Javier Escudero*<sup>1</sup>; <sup>1</sup>e-Xstream engineering

## Applications: Materials Design & Alloy Modification I

Tuesday AM  
April 26, 2022

Room: Martis Peak  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

8:00 AM Invited

**Accelerated ICME Design and Development of a New Single Crystal Ni Alloy with High Performance and Processibility:** *Jiadong Gong*<sup>1</sup>; <sup>1</sup>QuesTek Innovations LLC

8:30 AM

**Alloy Design Using Integrated High-Throughput Additive Manufacturing, Characterization, and Computation:** *Olivia Dippo*<sup>1</sup>; Kevin Kaufmann<sup>1</sup>; Kenneth Vecchio<sup>1</sup>; <sup>1</sup>University of California, San Diego

8:50 AM

**Accelerated HEA Development and Evaluation via Combined Approach of Additive Manufacturing, Machine Learning, and Thermodynamic Modeling:** *Phalgun Nelaturu*<sup>1</sup>; Jason Hattrick-Simpers<sup>2</sup>; Thien Duong<sup>3</sup>; Michael Moorehead<sup>1</sup>; Santanu Chaudhuri<sup>2</sup>; Adrien Couet<sup>1</sup>; Dan Thoma<sup>1</sup>; <sup>1</sup>University of Wisconsin; <sup>2</sup>National Institute of Standards and Technology; <sup>3</sup>Argonne National Laboratory

## Applications: Materials Design & Alloy Modification II

Tuesday AM  
April 26, 2022

Room: Martis Peak  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

10:40 AM Invited

**Design of an Austenitic Steel Weldment System Using ICME:** *Daniel Bechetti*<sup>1</sup>; Paul Lambert<sup>1</sup>; Matthew Sinfield<sup>1</sup>; Charles Fisher<sup>1</sup>; <sup>1</sup>Naval Surface Warfare Center, Carderock Division

11:10 AM

**Data-driven Design, Discovery, and Development (D5)<sup>TM</sup> of Novel Corrosion-Resistant Coating Alloys for Galvanizing of New Advanced High Strength Steels (AHSS):** *Rohit Bardapurkar*<sup>1</sup>; Christopher Borg<sup>2</sup>; John Speer<sup>1</sup>; Sridhar Seetharaman<sup>1</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Citrine Informatics

11:30 AM

**CALPHAD-Guided Alloy Design and Processing Approach for Strong and Tough Titanium Boride Based Ceramics & Composites:** *K. S. Ravi Chandran*<sup>1</sup>; Jun Du<sup>1</sup>; Ahmed Deghna<sup>1</sup>; <sup>1</sup>University of Utah

## Microstructure Evolution and Analysis I

Tuesday AM  
April 26, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

8:00 AM Invited

**Measurement of Flow Stresses at High Strain Rates and Temperatures for Improved Simulation of Friction Stir Welding:** John Prymak<sup>1</sup>; Kennen Brooks<sup>1</sup>; *Michael Miles*<sup>1</sup>; Tracy Nelson<sup>1</sup>; <sup>1</sup>Brigham Young University

8:30 AM

**Generation of Large-Scale Three-Dimensional Microstructures from Surface Images: Application to Additive Manufacturing:** *Iman Javaheri*<sup>1</sup>; Veera Sundararaghavan<sup>2</sup>; <sup>1</sup>NASA Langley Research Center; <sup>2</sup>University of Michigan

8:50 AM

**Object-Oriented Finite-Elements for Materials Science:** *Andrew Reid*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

9:10 AM

**Large Volume Grain Statistics with Laboratory Diffraction Contrast Tomography:** *Erik Lauridsen*<sup>1</sup>; *Jette Oddershede*<sup>1</sup>; *Jun Sun*<sup>1</sup>; *Hrishikesh Bale*<sup>2</sup>; *Florian Bachmann*<sup>1</sup>; <sup>1</sup>Xnovo Technology; <sup>2</sup>Carl Zeiss X-ray Microscopy Inc

9:30 AM

**Templated Product-Phase Microstructure via Directed Solid-State Synthesis: A Combined Mesoscale Modeling and Machine-Learning Approach:** *Connor McNamara*<sup>1</sup>; *Helen Chan*<sup>1</sup>; *Jeffrey Rickman*<sup>1</sup>; <sup>1</sup>Lehigh University

9:50 AM

**Modeling Magnetic Field Influence on Iron Alloy Phase Transformations:** *Heather Murdoch*<sup>1</sup>; *Efrain Hernandez*<sup>1</sup>; *Matthew Guziewski*<sup>1</sup>; *Anit Giri*<sup>1</sup>; *Daniel Field*<sup>1</sup>; <sup>1</sup>U.S. Army Research Laboratory

10:10 AM Break

## Microstructure Evolution and Analysis II

Tuesday AM  
April 26, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

10:30 AM

**Multiscale Model for Colony Breakdown Prediction in Two-Phase Titanium Alloys:** *Benjamin Begley*<sup>1</sup>; *Victoria Miller*<sup>1</sup>; <sup>1</sup>University of Florida

10:50 AM

**Phase Field Modelling of Microstructural Evolution in Double-Soaked Medium-Manganese Steels:** *Josh Mueller*<sup>1</sup>; *Alexandra Glover*<sup>2</sup>; *John Speer*<sup>1</sup>; *Emmanuel De Moor*<sup>1</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Los Alamos National Laboratory

11:10 AM

**Sharp Phase-Field Modeling of  $\gamma$ " Microstructure Evolution in Ni-base Superalloys:** *Felix Schleifer*<sup>1</sup>; *Yueh-Yu Lin*<sup>1</sup>; *Michael Fleck*<sup>1</sup>; *Uwe Glatzel*<sup>1</sup>; <sup>1</sup>University of Bayreuth

11:30 AM

**Microstructure-Sensitive Thermomechanical Forming Simulation Capability:** *Alexander Staroselsky*<sup>1</sup>; *Luke Borkowski*<sup>1</sup>; *Masoud Anahid*<sup>1</sup>; <sup>1</sup>Raytheon Technologies

## Multi-Scale Modeling I

Tuesday AM  
April 26, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

8:00 AM Invited

**First-Principles Statistical Mechanics to Connect Electronic Structure to Materials Properties at Meso and Macroscopic Scales:** *Anton Van der Ven*<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

8:30 AM

**Multiscale Thermal Conductivity Modeling of 3D Woven Composite Thermal Protection System Materials:** *Brett Bednarczyk*<sup>1</sup>; *Trenton Ricks*<sup>1</sup>; *Evan Pineda*<sup>1</sup>; *Subodh Mital*<sup>1</sup>; *Pappu Murthy*<sup>1</sup>; *Zhong Hu*<sup>2</sup>; <sup>1</sup>NASA Glenn Research Center; <sup>2</sup>South Dakota State University

8:50 AM

**Size Effects in Nano-Reinforced Polymers; from Interfacial Interactions to Bulk Properties:** *Fahmi Bedoui*<sup>1</sup>; *Andres Jaramillo-Botero*<sup>2</sup>; *William A. Goddard III*<sup>2</sup>; <sup>1</sup>Sorbonne Uiversité - Université de Technologie de Compiègne; <sup>2</sup>Materials and Process Simulation Center, CalTech

9:10 AM

**Microstructure Evolution During Multi-Stand Hot Rolling:** *Vitesh Shah*<sup>1</sup>; *Cornelis Bos*<sup>2</sup>; *Martin Diehl*<sup>1</sup>; *Franz Roters*<sup>1</sup>; <sup>1</sup>Max Planck Institute fuer Eisenforschung; <sup>2</sup>Tata Steel Europe

9:30 AM

**Fenics-Fracture: Phase-Field Modeling of Ductile Fracture with FENICS:** *Fabio Di Gioacchino*<sup>1</sup>; *Kester Clarke*<sup>1</sup>; *John Speer*<sup>1</sup>; <sup>1</sup>ASPPRC Colorado School of Mines

9:50 AM

**The PRISMS-PF Phase-Field Modeling Framework: Applications and Integration with Other PRISMS Computational Frameworks:** *David Montiel*<sup>1</sup>; *Stephen DeWitt*<sup>1</sup>; *Zhenjie Yao*<sup>2</sup>; *Yanjun Lyu*<sup>4</sup>; *Katsuyo Thornton*<sup>1</sup>; *John Allison*<sup>1</sup>; <sup>1</sup>University of Michigan

10:10 AM Break

## Multi-Scale Modeling II

Tuesday AM  
April 26, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

10:30 AM

**First Principles Prediction of Al-Cu, Al-Li and Al-Cu-Li Phase Diagrams:** *Sha Liu*<sup>1</sup>; *Wei Shao*<sup>2</sup>; *Javier Llorca*<sup>2</sup>; <sup>1</sup>IMDEA Materials Institute; <sup>2</sup>Universidad Politécnica de Madrid & IMDEA Materiales Institute

10:50 AM

**Formation of Crystalline Defects in Rapid Solidification:** *Tatu Pinomaa*<sup>1</sup>; *Sami Majaniemi*<sup>1</sup>; *Matti Lindroos*<sup>1</sup>; *Nikolas Provatas*<sup>2</sup>; *Anssi Laukkanen*<sup>1</sup>; <sup>1</sup>VTT Technical Research Centre of Finland; <sup>2</sup>McGill University

11:10 AM

**Using CASM for Development of Computational Software Tools:** *Brian Puchala*<sup>1</sup>; *John Thomas*<sup>2</sup>; *John Goiri*<sup>2</sup>; *Anton Van der Ven*<sup>2</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>University of California, Santa Barbara

11:30 AM

**Investigation of Liquid-Assisted Void Healing in Solders:** *Georg Siroky*<sup>1</sup>; *Elke Kraker*<sup>2</sup>; *Dietmar Kieslinger*<sup>3</sup>; *Ernst Kozeschnik*<sup>4</sup>; *Werner Ecker*<sup>2</sup>; <sup>1</sup>Technical University Vienna / Materials Center Leoben; <sup>2</sup>Materials Center Leoben Forschung GmbH; <sup>3</sup>ZKW Electronics GmbH; <sup>4</sup>Technical University Vienna

## Tuesday Plenary

Tuesday PM  
April 26, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

12:00 PM Plenary

**Virtual Testing of Structural Composites: A Multiscale Perspective:** *Carlos Gonzalez*<sup>1</sup>; <sup>1</sup>Imdea Materials Institute

12:30 PM Lunch



**1:30 PM Plenary**

**Hybrid Twin – Combining Physics- and Data-Based Models in a Consistent Digital Thread Spanning the AM Process Chain:** Monica Salgueiro<sup>1</sup>; Marcos Diez<sup>2</sup>; Camilo Prieto<sup>1</sup>; Bernardo Freire<sup>2</sup>; Mihail Babcsinski<sup>2</sup>; *Mustafa Megahed*<sup>3</sup>; <sup>1</sup>AIMEN; <sup>2</sup>University of Coimbra; <sup>3</sup>ESI Group

**2:10 PM Plenary**

**Computational Design of Lithium-ion Batteries Using Multi-Scale Models and Machine Learning:** *Kandler Smith*<sup>1</sup>; <sup>1</sup>National Renewable Energy Laboratory

**2:50 PM Break****3:10 PM Plenary**

**Accelerating the Broad Implementation of Verification and Validation in Computational Models of the Mechanics of Materials and Structures: A Science and Technology Accelerator Study:** Michael Tonks<sup>1</sup>; *George Spanos*<sup>2</sup>; <sup>1</sup>University of Florida; <sup>2</sup>TMS

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### Applications: Advanced Manufacturing – Additive Manufacturing III

Tuesday PM  
April 26, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

*Session Chairs:* TBD

**3:50 PM**

**Design by Fluid Flow Science for Multi-Metals Additive Manufacturing:** *Chinnapat Panwisawas*<sup>1</sup>; Junji Shinjo<sup>2</sup>; <sup>1</sup>University of Leicester; <sup>2</sup>Shimane University

**4:10 PM**

**Towards to an ICME Approach for the Discovery of Lightweight High Entropy Alloys:** *Shengyen Li*<sup>1</sup>; Jianliang Lin; John Macha; Mirella Vargas; Michael Miller; <sup>1</sup>Southwest Research Institute

**4:30 PM**

**The ExaAM AM Process-Aware Material Model:** *James Belak*<sup>1</sup>; John Turner<sup>2</sup>; ExaAM Team<sup>3</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>LLNL, LANL, ORNL

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### Artificial Intelligence & Machine Learning II

Tuesday PM  
April 26, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

*Session Chairs:* TBD

**3:50 PM**

**Machine Learning with Real-World Micrographs: A Study of Data Quality and Model Robustness:** *Xiaoting Zhong*<sup>1</sup>; Keenan Eves<sup>1</sup>; Brian Gallagher<sup>1</sup>; Yong-Jin Han<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

**4:10 PM**

**Discovery of Novel High-Entropy Ceramics via Machine Learning:** Kevin Kaufmann<sup>1</sup>; William Mellor<sup>1</sup>; Olivia Dippo<sup>1</sup>; *Kenneth Vecchio*<sup>1</sup>; <sup>1</sup>University of California, San Diego

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### Wednesday Plenary

Wednesday AM  
April 27, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

*Session Chairs:* TBD

**8:00 AM Plenary**

**Organizational Implementation of ICME in the Laboratory:** *Charles Ward*<sup>1</sup>; <sup>1</sup>Materials and Manufacturing Directorate, Air Force Research Laboratory

**8:40 AM Plenary**

**MPMD ICME Industry Implementation Award Recipient - ICME for High Strength Metal Alloys: Current Status and Future Challenges:** *Louis Hector*<sup>1</sup>; Anil Sachdev<sup>1</sup>; <sup>1</sup>General Motors Global Technical Center

**9:20 AM Plenary**

**Experimentalists in Quarantine: Building ICME Infrastructure and Talent Pipelines:** *Victoria Miller*<sup>1</sup>; <sup>1</sup>University of Florida

**10:00 AM Break**


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### Material Databases & Platforms I

Wednesday AM  
April 27, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

*Session Chairs:* TBD

**10:30 AM Invited**

**Exploring the Role of Uncertainty Quantification in Thermodynamic Data and Models:** *Noah Paulson*<sup>1</sup>; Joshua Gabriel<sup>1</sup>; Thien Duong<sup>1</sup>; Marius Stan<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

**11:00 AM**

**FAIR Digital Object Framework and Materials Science and Engineering:** *Zachary Trautt*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**11:20 AM**

**Holistic Integration of Experimental and Computational Approaches and Data for Rapid Establishment of Diffusion Databases for ICME:** *Ji-Cheng Zhao*<sup>1</sup>; Wei Zhong<sup>1</sup>; <sup>1</sup>University of Maryland

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### Multi-Scale Modeling III

Wednesday AM  
April 27, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

*Session Chairs:* TBD

**10:30 AM Invited**

**An Integrated Recursive Framework for Arbitrarily Multiscale and Multi-fidelity Modeling:** *Evan Pineda*<sup>1</sup>; Trenton Ricks<sup>1</sup>; Brett Bednarczyk<sup>1</sup>; Steven Arnold<sup>1</sup>; <sup>1</sup>NASA Glenn Research Center

**11:00 AM**

**Phonon Based Universal Sampling Method for Machine Learning Interatomic Potentials:** *Nathan Wilson*<sup>1</sup>; Xiaofeng Qian<sup>1</sup>; Raymundo Arroyave<sup>1</sup>; <sup>1</sup>Texas A&M University

**11:20 AM**

**Machine Learning Feature Selection for Predicting Corrosion Rates In High-Entropy Alloys:** *Mohammad Fuad Nur Taufique*<sup>2</sup>; Ankit Roy<sup>2</sup>; Ganesh Balasubramanian<sup>2</sup>; Gaoyuan Ouyang<sup>3</sup>; Duane Johnson<sup>3</sup>; Ram Devanathan<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Lehigh University; <sup>3</sup>Ames Laboratory

11:40 AM

**Bridging High-Fidelity and Macroscopic Simulations of the Laser Powder Bed Fusion Processes:** *Raeita Mehraban Teymour<sup>1</sup>; Chinnapat Panwisawas<sup>2</sup>; Bahram Ravani<sup>1</sup>; <sup>1</sup>University of California, Davis; <sup>2</sup>University of Leicester*

12:00 PM

**Multi-Scale Simulations of Crystallographic Facet-Oriented Dependent Corrosion Behavior in Metallic Alloys:** *Rongpei Shi<sup>1</sup>; Stephen Weitzner<sup>1</sup>; Tim Hsu<sup>1</sup>; Xiao Chen<sup>1</sup>; Tae Wook Heo<sup>1</sup>; Tuan Pham<sup>1</sup>; Christine Orme<sup>1</sup>; Morris Wang<sup>1</sup>; Brandon Wood<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory*

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### ICME Tools Workshops

Wednesday PM  
April 27, 2022

Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

1:30 PM Room: Regency Ballroom AB  
**PRISMS-Plasticity (Crystal Plasticity Finite Element):**  
Mohammadreza Yaghoobi<sup>1</sup>; <sup>1</sup>University of Michigan

1:30 PM Room: Martis Peak  
**Intro: Bayesian Optimization:** Raymundo Arroyave<sup>1</sup>; <sup>1</sup>Texas A&M University

1:30 PM Room: Regency Ballroom DE  
**LAMMPS (Molecular Dynamics):** Steve Plimpton<sup>1</sup>; <sup>1</sup>Sandia National Laboratories

2:00 PM Room: Martis Peak  
**BAREFOOT (Bayesian framework for materials optimization including data fusion):** Brent Vela<sup>1</sup>; <sup>1</sup>Texas A&M University

3:00 PM Break

3:20 PM Room: Regency Ballroom AB  
**PRISMS-PF (Phase Field):** David Montiel<sup>1</sup>; <sup>1</sup>University of Michigan

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### ICME for Non-Metals, Structural Composites, and Ceramics

Thursday AM  
April 28, 2022

Room: Regency Ballroom AB  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

9:00 AM Invited  
**Implementing Reactive Molecular Dynamics Simulations to Predict Residual Stresses in Polymers Using ICME:** Sagar Patil<sup>1</sup>; Khatereh Kashmari<sup>1</sup>; Sagar Shah<sup>2</sup>; Prathamesh Deshpande<sup>1</sup>; *Gregory Odegard<sup>1</sup>; Marianna Maiaru<sup>2</sup>; <sup>1</sup>Michigan Technological University; <sup>2</sup>University of Massachusetts Lowell*

9:30 AM

**Molecular Dynamics Simulation-Based Polymer Matrix Composite Model:** *Xiawa Wu<sup>1</sup>; <sup>1</sup>Penn State Behrend*

9:50 AM

**Multi-Objective Optimization of CALPHAD and Empirical Models to Discover New High-Temperature metallic Glasses:** *Jerry Howard<sup>1</sup>; Krista Carlson; Leslie Mushongera; <sup>1</sup>University of Nevada, Reno*

10:10 AM

**Process Modeling of Virtually Reconstructed Composites with ICME:** Sagar Shah<sup>1</sup>; *Marianna Maiaru<sup>1</sup>; <sup>1</sup>University of Massachusetts Lowell*

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### Material Databases & Platforms II

Thursday AM  
April 28, 2022

Room: Regency Ballroom DE  
Location: Hyatt Regency Lake Tahoe

Session Chairs: TBD

9:00 AM Invited

**Holistic Approaches to Establish Diffusion Mobility Databases for ICME Kinetics Simulations:** *Wei Zhong<sup>1</sup>; Ji-Cheng Zhao<sup>1</sup>; <sup>1</sup>University of Maryland*

9:30 AM

**New Open-Source Tools to Support a Robust ICME Infrastructure for Engineering the Mesoscale:** *Victoria Miller<sup>1</sup>; Benjamin Begley<sup>1</sup>; <sup>1</sup>University of Florida*

9:50 AM

**Atomistic Simulation and Calculation of Interfacial Properties of Fe, Fe<sub>3</sub>Al<sub>8</sub>, and FeZn<sub>13</sub> in Galvanized Steels:** *Kefan Chen<sup>1</sup>; Sungkwang Mun<sup>2</sup>; Bin Li<sup>1</sup>; Imran Aslam<sup>2</sup>; Michael Baskes<sup>3</sup>; Alexander Goldman<sup>1</sup>; <sup>1</sup>University of Nevada, Reno; <sup>2</sup>Mississippi State University; <sup>3</sup>University of North Texas*

10:10 AM

**The Materials Commons 2.0: Findable, Accessible, Understandable Materials Data:** *Brian Puchala<sup>1</sup>; Glenn Tarcea<sup>1</sup>; Tracy Berman<sup>1</sup>; John Allison<sup>1</sup>; <sup>1</sup>University of Michigan*

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### Poster Session

Monday & Tuesday PM  
April 25 & 26, 2022

Room: Regency Ballroom CF  
Location: Hyatt Regency Lake Tahoe

**Computational Fluid Dynamic Analysis to Evaluate Coating Film Thickness During Dip Coating Process:** *Rahman Ansari<sup>1</sup>; Jayendiran Raja<sup>1</sup>; Venkateswaran Perumal<sup>1</sup>; Dermot Dunne<sup>1</sup>; Cyril Tuohy<sup>1</sup>; <sup>1</sup>Stryker Global Technology Center*

**Computational Study of Li-Ion Conduction Mechanisms in Solid Electrolytes:** *Santosh Kc<sup>1</sup>; Ipsita Shahoo<sup>1</sup>; Dirar Mashaleh<sup>1</sup>; Gustavo Isarraras<sup>1</sup>; <sup>1</sup>San Jose State University*

**In-situ Testing to Acquire HR EBSD and DIC Strain Data within a Coincident Domain:** *Will Gilliland<sup>1</sup>; Sam Poulton<sup>1</sup>; Timothy Ruggles<sup>2</sup>; Geoffrey Bomarito<sup>3</sup>; Andrew Cannon<sup>4</sup>; Jacob Hochhalter<sup>1</sup>; <sup>1</sup>University of Utah; <sup>2</sup>Sandia National Laboratories; <sup>3</sup>National Aeronautics and Space Administration; <sup>4</sup>1900 Engineering LLC; Clemson University*

**Machine Learning Based Hierarchical Multiscale Modeling of Mechanical Deformation for Metal-Matrix-Nanocomposites:** *Md Shahrier Hasan<sup>1</sup>; Wenwu Xu<sup>1</sup>; Gregory Berkeley<sup>1</sup>; <sup>1</sup>San Diego State University*

**Numerical Simulation and Analysis of Solid Phase Processing: A Validated Friction Extrusion Smoothed Particle Hydrodynamics Model:** *Lei Li<sup>1</sup>; Xiao Li<sup>1</sup>; Anthony Reynolds<sup>2</sup>; Glenn Grant<sup>1</sup>; Ayoub Soulami<sup>1</sup>; <sup>1</sup>Battle Pacific Northwest National Laboratory; <sup>2</sup>University of South Carolina*

**ZEISS ZEN Intellesis - a Powerful and Open Machine Learning Ecosystem for Materials Microscopy:** *Tobias Volkenandt<sup>1</sup>; Robin White<sup>2</sup>; William Harris<sup>2</sup>; <sup>1</sup>Carl Zeiss Microscopy GmbH; <sup>2</sup>Carl Zeiss Microscopy LLC*

**Process Modeling of Cure in Epoxy Based Polymer Matrix Composites Using ICME:** *Prathamesh Deshpande<sup>1</sup>; Sagar Shah<sup>2</sup>; Sagar Patil<sup>1</sup>; Michael Olaya<sup>2</sup>; Gregory Odegard<sup>1</sup>; Marianna Maiaru<sup>2</sup>; <sup>1</sup>Michigan Technological University; <sup>2</sup>University of Massachusetts Lowell*

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

**Structure-Property (Small Punch Creep Rupture) Relationships in Low Carbon Steels:** *Johan Westraadt*<sup>1</sup>; <sup>1</sup>Nelson Mandela University

**Deformation Mechanisms of Additively Manufactured FeMnCoCrAl High Entropy Alloy with Interstitial Carbon - ICME Approach:** *Tommi Suhonen*<sup>1</sup>; Matti Lindroos<sup>1</sup>; Anssi Laukkanen<sup>1</sup>; Jarkko Metsajoki<sup>1</sup>; Ivanchenko Mykola<sup>1</sup>; Juha Lagerbom<sup>1</sup>; <sup>1</sup>VTT Technical Research Centre of Finland

**Calculation of Initial Stage of Solidified Shell Deformation During to  $\delta$  Transformation in Continuous Casting Mold of Steel:** *Kohei Furumai*<sup>1</sup>; Andre Phillion<sup>2</sup>; Hatem Zurob<sup>2</sup>; <sup>1</sup>JFE Steel; <sup>2</sup>McMaster University

**Materials Data Management to Meet Additive Manufacturing Requirements:** *Philippe Hebert*<sup>1</sup>; <sup>1</sup>Hexagon Manufacturing Intelligence

**Microstructure Classification and Quantification Method for Regular SEM Images of Complex Steel Microstructures Combining EBSD Labeling and Deep Learning:** *Chunguang Shen*<sup>1</sup>; *Chenrong Wang*<sup>1</sup>; *Wei Xu*<sup>1</sup>; <sup>1</sup>Northeastern University

**Fabrication of Precise Functionally Graded Materials (FGMs) via Directed Energy Deposition (DED):** *Kevin Luo*<sup>1</sup>; *Melanie Lang*; <sup>1</sup>FormAlloy

**Numerical Study on a Heat Transfer Model in the Solid-Carbon/Liquid-Copper-Silicon System:** *Khurram Iqbal*<sup>1</sup>; *Attria Ali*<sup>1</sup>; <sup>1</sup>Institute of Business Management (IoBM)

**Prediction of Rubber Failures Properties: Effects of Aging:** *Reda Kadri*<sup>1</sup>; *Moussa Nait Abdelaziz*<sup>1</sup>; *Bruno Fayolle*<sup>2</sup>; *Mouna Ben Hassine*<sup>3</sup>; *Yannick Nziakou Djouguela*<sup>3</sup>; *Julien Sanahuja*<sup>3</sup>; <sup>1</sup>University of Lille; <sup>2</sup>Arts et Métiers ParisTech; <sup>3</sup>Electricité de France

**Investigation of Time and Temperature Dependency of Cavitation Resistance of Al and Mg with Nonequilibrium Vacancy Concentrations:** *Sara Adibi*<sup>1</sup>; *Justin Wilkerson*<sup>2</sup>; <sup>1</sup>Mississippi State University, Center for Advanced Vehicular Systems; <sup>2</sup>Texas A&M University

**Fatigue Strength Prediction and High-Throughput Design by Mechanics Theory Guided Transfer Learning for Extremely Small Sample Database of Steels:** *Xiaolu Wei*<sup>1</sup>; *Chenrong Wang*<sup>1</sup>; *Chunguang Shen*<sup>1</sup>; *Wei Xu*<sup>1</sup>; <sup>1</sup>Northeastern University

**Hybrid Quantum-Classical Simulations of Metal Corrosion in Aqueous Environments:** *Stephen Weitzner*<sup>1</sup>; *Lisa Eggart*<sup>2</sup>; *Tuan Anh Pham*<sup>1</sup>; *Brandon Wood*<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Michigan Technological University

**Importance of Silica Hydroxylation in Ampyra Adsorption: DFT Study:** *A Diaz Compañy*<sup>1</sup>; *G Roman*<sup>1</sup>; *E Nosedá Grau*<sup>1</sup>; *S Simonetti*<sup>1</sup>; <sup>1</sup>IFISUR-UNS, UTN

**Integrated Simulation of the Heat Treatment and Calculation of the Load Bearing Capacity of Sintered Gears:** *Ali Rajaei*<sup>1</sup>; *Bengt Hallstedt*<sup>1</sup>; *Christoph Broeckmann*<sup>1</sup>; <sup>1</sup>IWM of RWTH Aachen University

**Residual Heat Effect on the Melt Pool Geometry During the Laser Powder Bed Fusion Process:** *Subin Shrestha*<sup>1</sup>; *Kevin Chou*<sup>1</sup>; <sup>1</sup>University of Louisville

**A Thermo-Mechanical Model for Prediction of Residual State during Wire Arc Additive Manufacturing (WAAM):** *Sami Hilal*<sup>1</sup>; *Djamel Missoum-Benziane*<sup>1</sup>; *Pierre Kerfriden*<sup>1</sup>; *Sofiane Hendili*<sup>2</sup>; *Matthieu Maziere*<sup>1</sup>; <sup>1</sup>Centre des Matériaux-Mines Paristech; <sup>2</sup>EDF R&D Division

**Design of Stable Nanocrystalline Aluminum by Evolutionary Computation:** *Jake Hohl*<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

**ICME Framework to Predict the Precipitation Kinetics and Microstructural Evolution of Hot-Rolled TRIP Steel:** *Pranjal Chauhan*<sup>1</sup>; *Vaibhav Malik*<sup>1</sup>; *Saurabh Kumar*<sup>1</sup>; *Surya Ardhama*<sup>2</sup>; *Himanshu Nirgudkar*<sup>2</sup>; *Akash Bhattacharjee*<sup>2</sup>; *Dinesh Nath*<sup>1</sup>; *Gerald Tennyson*<sup>2</sup>; *Amarendra Singh*<sup>1</sup>; <sup>1</sup>Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kanpur; <sup>2</sup>TCS Research, Tata Consultancy Services Limited, Pune

## On-Demand Oral Presentations

Monday AM  
May 2, 2022

Room: On-Demand Session Room  
Location: Hyatt Regency Lake Tahoe

**A Microstructure-Based Finite Element Modeling Approach to Predict the Mechanical Properties of Zircaloy with Hydride Precipitates:** *Shank Kulkarni*<sup>1</sup>; *Varun Gupta*<sup>2</sup>; *Timothy Truster*<sup>3</sup>; *David Senior*<sup>1</sup>; *Ram Devanathan*<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>ExxonMobil Upstream Research Company; <sup>3</sup>University of Tennessee Knoxville

**Understanding the Interplay between Orientation, Temperature and Lamellar Thickness of Fully Lamellar Titanium Aluminides: A Crystal Plasticity Finite Element Study:** *Balaji Selvarajou*<sup>1</sup>; *Quek Siu Sin*<sup>1</sup>; *Mark Jhon*<sup>1</sup>; *Raju Ramanujan*<sup>2</sup>; <sup>1</sup>Institute of High Performance Computing; <sup>2</sup>Nanyang Technological University

**Exploration of Microstructural Evolution for Aluminum Alloy Powders through In-Situ TEM and DICTRA Simulations:** *Kyle Tsaknopoulos*<sup>1</sup>; *Matthew Gleason*<sup>1</sup>; *Grace Fitzpatrick-Schmidt*<sup>1</sup>; *Danielle Cote*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

**Theoretical Model of the Flow Properties of Post Processed Direct Metal Laser Sintering Ti6Al4V:** *Amos Muiruri*<sup>1</sup>; *Maina Maringa*<sup>1</sup>; *Willie du Preez*<sup>1</sup>; <sup>1</sup>Central University of Technology, Free State

**A Multiscale Approach on Strategy to Mitigate Deformation Twinning in Magnesium Alloys:** *Yubraj Paudel*<sup>1</sup>; *Christopher Barrett*<sup>1</sup>; *Hongjoo Rhee*<sup>1</sup>; *Haitham EL Kadiri*<sup>1</sup>; <sup>1</sup>Mississippi State University

**A Static and Dynamic Recrystallization Internal State Variable Constitutive Model Based on Microstructures and Its History Effect:** *Heechen Cho*<sup>1</sup>; *Mark Horstemeyer*<sup>1</sup>; <sup>1</sup>Liberty University

## On-Demand Posters

Monday AM  
May 2, 2022

Room: On-Demand Session Room  
Location: Hyatt Regency Lake Tahoe

**Modeling of Grain Structure Development as a Function of Melt Pool Shape and Grid Resolution During Alloy AM:** *Matthew Rolchigo*<sup>1</sup>; *John Coleman*<sup>1</sup>; *Gerry Knapp*<sup>1</sup>; *Sam Reeve*<sup>1</sup>; *Robert Carson*<sup>2</sup>; *Jim Belak*<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Lawrence Livermore National Laboratory

**Analysis and Numerical Simulation of Plastic Anisotropy Behavior of DIN 1623 St14 Steel Sheet Under Associated Flow Rule Approach:** *Kaouter Babouri*<sup>1</sup>; *Nedjouda Matougui*<sup>1</sup>; *Oualid Chahaoui*<sup>1</sup>; <sup>1</sup>National School of Mining and Metallurgy-Annaba; <sup>2</sup>Engineering Sciences and Advanced Materials Laboratory (ISMA), Laghrour-Abbes University of Khenchela

**Analysis and Numerical Simulation of Microstructural Anisotropy Behavior of DIN 1623 St14 Steel Before and After Recrystallisation:** *Kaouter Babouri*<sup>1</sup>; *Nedjouda Matougui*<sup>1</sup>; *Oualid Chahaoui*<sup>1</sup>; <sup>1</sup>National School of Mining and Metallurgy-Annaba

**Image Processing Based Failure Site Prediction of PC Wires During Wiredrawing Using Supervised Machine Learning Approach:** *Mohamed Heddar<sup>1</sup>; Mehdi Brahim<sup>2</sup>; Nedjouda Matougui<sup>1</sup>; <sup>1</sup>ENSMM - Annaba; <sup>2</sup>CRTI - Cheraga*

**Study of Dendrite Growth in Nickel-Based Superalloy Directional Solidification via a GPU-Accelerated Multiphase-Field-Lattice Boltzmann Method:** *Xia Huxiang<sup>1</sup>; <sup>1</sup>Tsinghua University*

**Machine Learning Assisted Yield Strength and Hardness Prediction of Multi-Principal Element Alloys:** *Mohammad Fuad Nur Taufique<sup>1</sup>; Ankit Roy<sup>2</sup>; Ganesh Balasubramanian<sup>2</sup>; Gaoyuan Ouyang<sup>3</sup>; Duane Johnson<sup>3</sup>; Ram Devanathan<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Lehigh University; <sup>3</sup>Ames Laboratory*

**Molecular Dynamics Simulation of Adhesive Response to Aging for Epoxy Polymer:** *Mohammad Fuad Nur Taufique<sup>1</sup>; Martin Losada<sup>2</sup>; Nir Goldman<sup>3</sup>; Sebastien Hamel<sup>3</sup>; Ram Devanathan<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>PPG Industries, Inc. ; <sup>3</sup>Lawrence Livermore National Laboratory*

**Core Structure, Energy, and Mobility of Pyramidal Dislocations in Magnesium:** *Yang Yang<sup>1</sup>; Bin Li<sup>1</sup>; Kefan Chen<sup>1</sup>; <sup>1</sup>University of Nevada, Reno*

**Effect of Grain Boundary Migration on Radiation Induced Segregation in Polycrystalline Metal:** *Aashique Rezwani<sup>1</sup>; Yongfeng Zhang<sup>1</sup>; <sup>1</sup>University of Wisconsin Madison*

**Modeling of Coupled Diffusion Transport in Cylindrical Transformations:** *Rahul Basu<sup>1</sup>; <sup>1</sup>VTU*

**The Influence of Pore Defects on the Mechanical Behavior of Product Parts Using Micromechanics:** *Nannan Song; shenghua wu; Flavio Souza; Jeyachandran Rajesh<sup>1</sup>; Kedar Malusare<sup>2</sup>; <sup>1</sup>Siemens Digital Industries Software; <sup>2</sup>Siemens PLM Software*



A			
Adam, L	3	Cote, D	7
Adibi, S	2, 7	Couet, A	3
Agrawal, P	2	D	
Alekseyenko, A	2	Deghna, A	3
Ali, A	7	De Moor, E	4
Allison, J	2, 4, 6	Deshpande, P	6
Alman, D	2	Devanathan, R	2, 5, 7, 8
Anahid, M	4	DeWitt, S	4
Ansari, R	6	Diaz Compañy, A	7
Ardham, S	7	Dickel, D	2, 2
Arnold, S	5	Diehl, M	2, 4
Aroh, J	3, 7	Diez, M	5
Arroyave, R	5	Di Gioacchino, F	4
Aslam, I	6	Dippo, O	3, 5
B		Du, J	3
Babcinski, M	5	Dunne, D	6
Babouri, K	7	Duong, T	3, 5
Bachmann, F	4	du Preez, W	7
Bahloul, A	8	E	
Balasubramanian, G	5, 8	Ecker, W	4
Bale, H	4	Eggart, L	7
Bardapurkar, R	3	Eisenlohr, P	2
Barrett, C	7	El Kadiri, H	7
Baskes, M	6	Escudero, J	3
Basu, R	8	Eves, K	5
Bechetti, D	3	F	
Bednarczyk, B	4, 5	Fayolle, B	7
Bedoui, F	4	Field, D	4
Beets, B	3	Fisher, C	2, 3
Begley, B	4, 6	Fitzpatrick-Schmidt, G	7
Belak, J	2, 5, 7	Fleck, M	4
Ben Hassine, M	7	Frazier, W	3
Berkeley, G	6	Freire, B	5
Berman, T	6	Furumai, K	7
Berry, J	3	Fu, Y	3
Bhattacharjee, A	7	G	
Bian, L	2	Gabriel, J	5
Bocklund, B	3	Gallagher, B	5
Bomarito, G	6	Ganesan, S	2
Borg, C	3	Gao, M	3
Borkowski, L	4	Gerstner, K	2
Bos, C	4	Ghaffari, B	2
Brady, M	3	Gilliland, W	6
Brahim, M	8	Giri, A	4
Broeckmann, C	7	Glatzel, U	4
Brooks, K	3	Glavas, V	2
C		Glazoff, M	3
Campbell, C	3	Gleason, M	7
Cannon, A	6	Glover, A	4
Capolungo, L	2, 3	Goddard III, W	4
Carlson, K	6	Goiri, J	4
Carson, R	7	Goldman, A	6
Cerreta, E	2	Goldman, N	8
Chadwick, A	2	Gong, J	3
Chahaoui, O	7	Gonzalez, C	4
Chakraborty, A	3	Gopalakrishnan, S	2
Chandran, K	3	Gopman, D	3
Chan, H	4	Gould, B	7
Chauduri, S	3	Grant, G	6
Chauhan, P	7	Greeley, D	2
Chen, K	6, 8	Gupta, V	7
Chen, X	6	Guziewski, M	4
Cho, H	7		
Choi, K	3		
Chou, K	7		
Clarke, K	4		
Coleman, J	7		
		H	
		Hallstedt, B	7
		Hamel, S	8
		Han, Y	5
		Hareland, C	2
		Harris, W	6
		Hartman, N	2
		Hasan, M	6
		Hattrick-Simpers, J	3
		Hawk, J	2
		Hebert, P	7
		Hector, L	5
		Heddar, M	8
		Henderson, H	3
		Hendili, S	7
		Heo, T	6
		Hernandez, E	4
		Hilal, S	7
		Hochhalter, J	6
		Hohl, J	7
		Horstemeyer, M	7
		Howard, J	6
		Hsu, T	6
		Huang, S	2
		Huxiang, X	8
		Hu, Z	4
		I	
		Ilevbare, G	2
		Iqbal, K	7
		Isarraras, G	6
		J	
		Jaramillo-Botero, A	4
		Jasien, C	2
		Javaheri, I	3
		Jayaganthan, R	2
		Jhon, M	7
		Jiang, R	7
		Jiao, Y	2
		Johnson, D	5, 8
		Joshi, V	3
		Ju, S	2
		K	
		Kadri, R	7
		Kashmari, K	6
		Kaufmann, K	2, 3, 5
		Kc, S	6
		Kerfriden, P	7
		Kerwin, L	2
		Kieslinger, D	4
		Kitt, A	2
		Knapp, G	7
		Kozeschnik, E	4
		Kraker, E	4
		Kramer, M	2
		Kucheyev, S	2
		Kulkarni, S	7
		Kumar, A	3
		Kumar, S	7
		Kuna, L	2

L		Nziakou Djouguela, Y . . . . .	7	Senor, D . . . . .	7
Lagerbom, J . . . . .	7	O		Shahoo, I . . . . .	6
Lakshmanan, A . . . . .	2	Oddershede, J . . . . .	4	Shah, S . . . . .	6
Lambert, P . . . . .	3	Odegard, G . . . . .	6	Shah, V . . . . .	4
Landa, A . . . . .	3	Olaya, M . . . . .	6	Shanthraj, P . . . . .	2
Lane, H . . . . .	2	Orme, C . . . . .	6	Shao, W . . . . .	4
Lang, M . . . . .	7	Otis, R . . . . .	3	Shen, C . . . . .	2, 7
Lara-Curzio, E . . . . .	2	Ouyang, G . . . . .	5, 8	Shinjo, J . . . . .	5
Laukkanen, A . . . . .	4, 7	P		Shi, R . . . . .	6
Lauridsen, E . . . . .	4	Panwisawas, C . . . . .	5, 6	Shrestha, S . . . . .	7
Lavender, C . . . . .	3	Parolini, J . . . . .	2	Simonetti, S . . . . .	7
Lebensohn, R . . . . .	3	Patil, S . . . . .	6	Sims, Z . . . . .	3
Li, B . . . . .	6, 8	Paudel, Y . . . . .	7	Sinfield, M . . . . .	3
Li, L . . . . .	3, 6	Paulson, N . . . . .	5	Singh, A . . . . .	7
Lindroos, M . . . . .	4, 7	Pauza, J . . . . .	3	Siroky, G . . . . .	4
Lin, J . . . . .	5	Perron, A . . . . .	3	Siu Sin, Q . . . . .	7
Lin, Y . . . . .	4	Perumal, V . . . . .	6	Smith, K . . . . .	5
Li, S . . . . .	5	Pham, T . . . . .	6, 7	Song, H . . . . .	2
Liu, S . . . . .	4	Phillion, A . . . . .	7	Song, N . . . . .	8
Li, X . . . . .	6	Pineda, E . . . . .	4, 5	Soulami, A . . . . .	3, 6
Llorca, J . . . . .	4	Pinomaa, T . . . . .	4	Souly, N . . . . .	2
Lordi, V . . . . .	3	Pistorius, P . . . . .	3	Souza, F . . . . .	8
Losada, M . . . . .	8	Poulton, S . . . . .	6	Spanos, G . . . . .	5
Luo, K . . . . .	7	Priddy, M . . . . .	2	Speer, J . . . . .	3, 4
Lyu, Y . . . . .	4	Prieto, C . . . . .	5	Stan, M . . . . .	5
M		Prithvirajan, V . . . . .	3	Staroselsky, A . . . . .	4
Macha, J . . . . .	5	Provatas, N . . . . .	4	Stopka, K . . . . .	2
Maiaru, M . . . . .	6	Prymak, J . . . . .	3	Stoudt, M . . . . .	3
Majaniemi, S . . . . .	4	Puchala, B . . . . .	4, 6	Suhonen, T . . . . .	7
Malik, V . . . . .	7	Pyeon, J . . . . .	7	Sun, C . . . . .	2
Malusare, K . . . . .	8	Q		Sundararaghavan, V . . . . .	2, 3
Maringa, M . . . . .	7	Qian, X . . . . .	5	Sundar, S . . . . .	2
Mashaleh, D . . . . .	6	R		Sun, J . . . . .	4
Matougui, N . . . . .	7, 8	Raabe, D . . . . .	2	T	
MAZIERE, M . . . . .	7	Rajaei, A . . . . .	7	Tae, C . . . . .	2
McCall, S . . . . .	3	Raja, J . . . . .	6	Tang, G . . . . .	3
McDowell, D . . . . .	2	Rajesh, J . . . . .	8	Tarcea, G . . . . .	6
McKeown, J . . . . .	3	Ramanujan, R . . . . .	7	Taufique, M . . . . .	5, 8
McNamara, C . . . . .	4	Ramlatchan, A . . . . .	7	Tavazza, F . . . . .	2
Megahed, M . . . . .	5	Ravani, B . . . . .	6	Team, E . . . . .	5
Mehraban Teymouri, R . . . . .	6	Reeve, S . . . . .	2, 7	Teferra, K . . . . .	2
Mellor, W . . . . .	5	Reid, A . . . . .	4	Tennyson, G . . . . .	7
Metsajoki, J . . . . .	7	Reynolds, A . . . . .	6	Thoma, D . . . . .	3
Miles, M . . . . .	3	Rezwan, A . . . . .	8	Thomas, J . . . . .	4
Miller, M . . . . .	5	Rhee, H . . . . .	7	Thornton, K . . . . .	4
Miller, V . . . . .	4, 5, 6	Rickman, J . . . . .	4	Tong, C . . . . .	3
Missoum-Benziane, D . . . . .	7	Ricks, T . . . . .	4, 5	Tonks, M . . . . .	5
Mital, S . . . . .	4	Rolchigo, M . . . . .	2, 7	Toth, M . . . . .	3, 8
Mohr, L . . . . .	2	Rollett, A . . . . .	3, 7	Trautt, Z . . . . .	5
Montiel, D . . . . .	4	Roman, G . . . . .	7	Truster, T . . . . .	7
Moorehead, M . . . . .	3	Roters, F . . . . .	2, 4	Tsaknopoulos, K . . . . .	7
M. R . . . . .	2	Rowenhorst, D . . . . .	2	Tuohy, C . . . . .	6
Mueller, J . . . . .	4	Roy, A . . . . .	5, 8	Turner, J . . . . .	5
Muiruri, A . . . . .	7	Rudraraju, S . . . . .	2	V	
Mun, S . . . . .	2, 6	Ruggles, T . . . . .	6	Van der Ven, A . . . . .	4
Murdoch, H . . . . .	4	S		Vargas, M . . . . .	5
Murthy, P . . . . .	4	Sachdev, A . . . . .	5	Vecchio, K . . . . .	2, 3, 5
Mushongera, L . . . . .	6	Salgueiro, M . . . . .	5	Venkataramana, M . . . . .	2
Mykola, I . . . . .	7	Samanta, A . . . . .	3	Voisin, T . . . . .	3
N		Sanahuja, J . . . . .	7	Volkenandt, T . . . . .	6
Nait Abdelaziz, M . . . . .	7	Sangid, M . . . . .	2	Voorhees, P . . . . .	2
Nath, D . . . . .	7	Schleifer, F . . . . .	4	W	
Negoita, A . . . . .	2	Seetharaman, S . . . . .	3	Wang, C . . . . .	7
Nelaturu, P . . . . .	3	Selvarajou, B . . . . .	7	Wang, M . . . . .	6
Nelson, T . . . . .	3				
Nirgudkar, H . . . . .	7				
Nosedo Grau, E . . . . .	7				

Ward, C	5
Wegener, J	2
Weitzner, S	6, 7
Wei, X	7
Wen, Y	3
Westraadt, J	7
White, R	6
Wilkerson, J	7
Williams, M	3
Wilson, N	5
Wong, G	3
Wood, B	6, 7
wu, s	8
Wu, X	6
X	
Xu, W	6, 7
Xu, Z	3
Y	
Yaghoobi, M	2
Yamamoto, Y	3
Yang, Y	8
Yao, Z	4
Yuan, L	2
Z	
Zhang, Y	2, 8
Zhao, J	5, 6
Zhong, W	5, 6
Zhong, X	5
Zhu, C	2
Zuback, J	3
Zurob, H	7