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The Minerals, Metals & Materials Society



## 3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)

May 31–June 4, 2015 • Cheyenne Mountain Resort  
Colorado Springs, Colorado, USA

# PROGRAM PREVIEW

Register by May 8, 2015 and save!

[www.tms.org/ICME2015](http://www.tms.org/ICME2015)



## REGISTER NOW for ICME 2015!

A key goal of ICME 2015 is to convene stakeholders from across areas of modeling, simulation, and experimental specialization, as well as from across academia, government, and industry to address the integration of tools and techniques and examine their application to engineering.

Integrated Computational Materials Engineering (ICME) is a methodology that can unlock the potential for large benefits in cost-effective, efficient materials and process design. Building on the successes of the TMS First and Second World Congresses, held in 2011 and 2013, respectively, this third installment (ICME 2015) intends to capture the current state-of-the-art, identify gaps in ICME efforts, and set the stage for continued growth and implementation of ICME worldwide.

### CONGRESS ORGANIZERS

#### Organizing Committee:

**Chair:** Warren Poole, *University of British Columbia, Canada*

Steve Christensen, *Boeing, USA*

Surya Kalidindi, *Georgia Institute of Technology, USA*

Alan Luo, *Ohio State University, USA*

Jonathan Madison, *Sandia National Laboratories, USA*

Dierk Raabe, *Max-Planck Institute, Germany*

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#### International Advisory Committee:

John Ågren, *KTH - Royal Institute of Technology, Sweden*

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Mei Li, *Ford Motor Company, USA*

Baicheng Liu, *Tsinghua University, China*

Jiang-Feng Nie, *Monash University, Australia*

Tresa Pollock, *University of California Santa Barbara, USA*

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Gary Purdy, *McMaster University, Canada*

Alejandro Strachan, *Purdue University, USA*

Anthony Waas, *University of Michigan, USA*

James Warren, *National Institute of Standards and Technology, USA*

### REGISTRATION

All congress attendees, including authors, presenters, and session chairs, are required to register. To receive the discount registration rate, register at [www.tms.org/ICME2015](http://www.tms.org/ICME2015) by May 8, 2015.

Registration Fees	Discount*	Standard
Member	\$695	\$795
Nonmember**	\$825	\$925
Student Member*	\$450	\$450
Student Nonmember*	\$525	\$525

+ Includes TMS membership for 2015.

\* Discount rates apply through May 8, 2015.

\*\* A copy of student school identification card must accompany registration form.

#### Registration package includes:

- One copy of the congress proceedings
- Technical sessions
- Refreshment breaks
- Welcome reception
- Poster receptions
- Congress dinner
- One copy of "Modeling Across Length Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales"

### LOCATION, HOUSING & TRAVEL

#### Congress Location—Cheyenne Mountain Resort

For information, visit  
[www.cheyennemountain.com](http://www.cheyennemountain.com).



Known for its breathtaking mountain views, exceptional accommodations, two restaurants and one lounge featuring Colorado fresh cuisine, a myriad of activities, and comprehensive conference facilities, the AAA Four Diamond Cheyenne Mountain Resort and Country Club offers the ultimate in Colorado vacationing. A vast array of amenities include an 18-hole championship, Pete Dye-designed golf course; five swimming pools; tennis courts; full-service fitness center; aquatics center; and a 35-acre recreation lake.

## Housing

A block of rooms has been reserved at the Cheyenne Mountain Resort at a special rate. Accommodations must be secured by May 8, 2015. Single/double occupancy is \$169 per night.

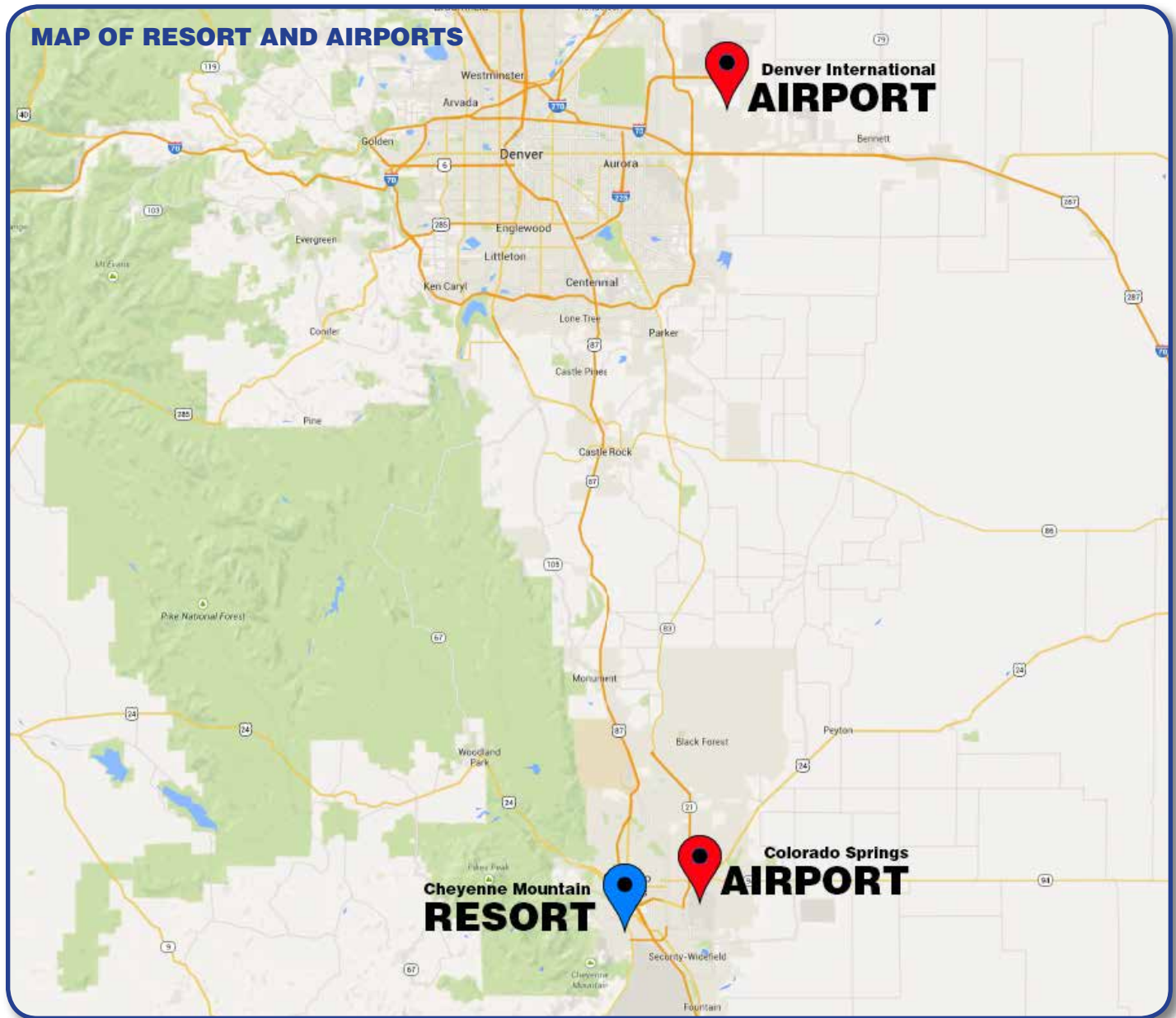
Visit [www.tms.org/ICME2015](http://www.tms.org/ICME2015) to make your reservations.

## Getting There

The Cheyenne Mountain Resort is a 20-minute drive from the Colorado Springs Airport and approximately a one-hour drive from the Denver International Airport. For more information on transportation and parking, visit [www.cheyennemountain.com](http://www.cheyennemountain.com).

## NETWORKING/SOCIAL EVENTS

Sunday, May 31	Monday, June 1
Welcome Reception 6:30 p.m. to 7:30 p.m. Colorado Gallery	Poster Viewing/ Reception 5:00 p.m. to 6:30 p.m. Colorado Ballroom I
Tuesday, June 2	Wednesday, June 3
Poster Viewing/ Reception 5:00 p.m. to 6:30 p.m. Colorado Ballroom I	Congress Dinner 6:00 p.m. to 8:00 p.m. Remington I & II



## TECHNICAL PROGRAM

ICME has emerged as an important discipline in recent years, due to its great potential in efficiently engineering new products and manufacturing processes. ICME methodologies can identify the gaps in the integration process when applied to solve fundamental engineering problems. This can lead to advancements in the fundamental understanding of the problems; development of the linkages along the processing chain; development of computational tools and advanced experimental techniques for engineering practice; and establishment of an infrastructure for global information sharing.

This congress will provide a forum for presenters and discussions centered on ICME-related topics, including:

- The wide range of materials programs where an ICME approach validated by experimental efforts is applicable, including computational- and experimental-based talks
- Individual computational methods utilized in an ICME approach, including both advantages and limitations
- Roles of ICME in graduate and undergraduate courses
- Digital infrastructure required for information sharing and model integration
- ICME implementation strategies
- Verification, validation, and uncertainty quantification issues

## SPONSORSHIP OPPORTUNITIES

Corporate sponsorship offers high visibility at the congress reception, refreshment breaks, and attendee social activities, as well as on registration amenities like reusable canvas bags, badges, and lanyards.

**For more information on purchasing a corporate sponsorship, visit the Sponsorship page of the ICME 2015 website: [www.tms.org/ICME2015](http://www.tms.org/ICME2015)**

### NEW for 2015: ICME TOOLS SHOWCASE

ICME 2015 organizers are offering exhibitors and sponsors the opportunity to showcase their company and products in a unique way to attendees: a tools showcase. The showcase, comprised of 10-minute presentations from participating companies, will be held during technical session hours on Tuesday, June 2. This amazing opportunity to directly address congress attendees in a presentation setting is included with the price of an exhibit table top. You must be an exhibitor or sponsor to take part in the showcase.

To learn more about how your company can participate, contact Caron Gavrish, Sales Specialist, at [cgavrish@tms.org](mailto:cgavrish@tms.org).

## Continue the ICME Discussion With “Implementing ICME in Industry”

June 4–5, 2015 • Cheyenne Mountain Resort • Colorado Springs, Colorado, USA

Immediately following ICME 2015 TMS will hold the “Implementing ICME in Industry” short course, built on key findings and recommendations of the 2013 TMS study, *Integrated Computational Materials Engineering (ICME): Implementing ICME in the Automotive, Aerospace, and Maritime Industries*. The course will cover frameworks for implementing ICME within the product development cycle, barriers and solutions to implementing ICME, making the business case for ICME, and much more. Instructors for this course are:



**John Allison**, University of Michigan and American Lightweight Metals Manufacturing Innovation Institute; *ICME Implementation Study—Automotive Team Leader*



**Rick Barto**, Lockheed Martin Advanced Technology Labs; *ICME Implementation Study—Aerospace Team*



**Mei Li**, Ford Research and Advanced Engineering Laboratory; *ICME Implementation Study—Automotive Team*

For more information on this course or the course instructors, view the [Short Course tab](#) on the ICME 2015 website. Advance registration for this course will end **May 8, 2015**. Short course registration is offered on the [ICME 2015 registration form](#) (conference registration is not required to attend the course).

## Monday, June 1, 2015

### Plenary Session I • Room: Colorado Ballroom II & III

- 8:00 AM **Invited**  
ICME: Past, Present and Future: John Allison
- 8:30 AM **Invited**  
Title to be Announced: Tresa Pollock<sup>1</sup>; <sup>1</sup>University of California Santa Barbara
- 9:00 AM **Question and Answer Period**
- 9:20 AM **Invited**  
Materials Genomics: From CALPHAD to Flight: Greg Olson<sup>1</sup>; <sup>1</sup>Northwestern University
- 9:40 AM **Invited**  
Multiscale Modeling of Phase Transformations in High-performance Steels: Matthias Militzer<sup>1</sup>; <sup>1</sup>The University of British Columbia
- 10:00 AM **Break**

### Applications I: Lightweight Materials • Room: Colorado Ballroom II & III

- 10:20 AM **Experiments and Modeling of Three-dimensional Dendritic Morphology of Magnesium Alloy:** Manhong Yang<sup>1</sup>; Zhipeng Guo<sup>1</sup>; Shou-Mei Xiong<sup>1</sup>; <sup>1</sup>Tsinghua University
- 10:40 AM **Sensitization Effects on the Fracture and Fatigue Crack Growth Behavior of Al-Mg Alloys:** Mohsen Seifi<sup>1</sup>; Bo Li<sup>1</sup>; John Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University
- 11:00 AM **Computer Simulations of Mg/Al Cladding Process by Twin-roll Casting:** Jong-Jin Park<sup>1</sup>; <sup>1</sup>Hongik University
- 11:20 AM **An Integrated Simulation Tool for Novel Mg and Al Alloy Design:** Manas Paliwal<sup>1</sup>; In-Ho Jung<sup>1</sup>; <sup>1</sup>McGill University
- 11:40 AM **Flat-Rolled Aluminum Production: Opportunities for Continued ICME Impact:** Babak Raeisina<sup>1</sup>; <sup>1</sup>Novelis Global R&T Center
- 12:00 PM **A Phase Field Simulation of the Recrystallization Process after High Temperature Deformations of Al-Mn-Fe-Si (AA3XXX) Alloys:** Jingqi Chen<sup>1</sup>; Benqiang Zhu<sup>1</sup>; Warren Poole<sup>1</sup>; <sup>1</sup>The University of British Columbia
- 12:20 PM **Lunch Break**

### Modeling at Different Scales I • Room: Arkansas/Platte

- 10:20 AM **Investigating Dislocation-vacancy Interactions at the Atomic Scale:** Lucas Hale<sup>1</sup>; Chandler Becker<sup>1</sup>; Zachary Trautt<sup>1</sup>; Jonathan Zimmerman<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>Sandia National Laboratories
- 10:40 AM **A Molecular Dynamics Simulation Mechanism with Imprecise Interatomic Potentials:** Anh Tran<sup>1</sup>; Yan Wang<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- 11:00 AM **Uncertainty Quantification and Sensitivity Analysis of Graphene's Property Prediction from Molecular Dynamics Simulations:** Tomas Mawzyin<sup>1</sup>; Chandra Veer Singh<sup>1</sup>; Prasanth Nair<sup>1</sup>; <sup>1</sup>University of Toronto
- 11:20 AM **First-principles Study of Interface between Iron and Precipitate:** Hideaki Sawada<sup>1</sup>; Shunsuke Taniguchi<sup>1</sup>; Kazuto Kawakami<sup>1</sup>; Taisuke Ozaki<sup>2</sup>; <sup>1</sup>Nippon Steel & Sumitomo Metal Corporation; <sup>2</sup>The University of Tokyo
- 11:40 AM **Prediction of Microstructure and Mechanical Properties in Aluminum High Pressure Die Castings after Heat Treatment:** Jianzheng Guo<sup>1</sup>; Sam Scott<sup>2</sup>; Weisheng Cao<sup>3</sup>; <sup>1</sup>ESI US R&D; <sup>2</sup>ESI NA; <sup>3</sup>Computherm LLC
- 12:00 PM **Multiscale Modeling of Thermal Protection Materials II: Micromechanical Modeling of Composite Performance:** Steven Arnold<sup>1</sup>; Pappu Murthy<sup>1</sup>; Brett Bednarczyk<sup>1</sup>; John Lawson<sup>1</sup>; Charles Bauschlicher<sup>1</sup>; Joshua Monk<sup>1</sup>; <sup>1</sup>NASA
- 12:20 PM **Lunch Break**

### Process and Performance Modeling I • Room: Rio Grande/Gunnison

- 10:20 AM **Direct Numerical Simulations in Solid Mechanics for Understanding the Engineering-scale Effects of Microstructure:** Joseph Bishop<sup>1</sup>; John Emery<sup>1</sup>; <sup>1</sup>Sandia National Laboratories
- 10:40 AM **Meso-Scale Predictions of Laser-Weld Microstructure via Kinetic Monte-Carlo Simulation:** Jonathan Madison<sup>1</sup>; Efrain Hernandez<sup>2</sup>; Veena Tikare<sup>1</sup>; <sup>1</sup>Sandia National Laboratories; <sup>2</sup>University of Michigan
- 11:00 AM **ICME Application in Optimizing Welding and Thermal-Forming Processes:** Yu-Ping Yang<sup>1</sup>; Hyunok Kim<sup>1</sup>; Bill Mohr<sup>1</sup>; Harvey Castner<sup>1</sup>; <sup>1</sup>EWI

- 11:20 AM **Resolving the Evolution of Pore Structures in 304-L Laser Welds Through Remeshing and Mapping of Internal State Variables:** *James Foulk*<sup>1</sup>; <sup>1</sup>Sandia National Laboratories
- 11:40 AM **Manufacturing and Evaluation of High Entropy Alloys:** Joseph Licavoli<sup>1</sup>; *Paul Jablonski*<sup>1</sup>; Michael Gao<sup>1</sup>; Jeff Hawk<sup>1</sup>; <sup>1</sup>Department of Energy
- 12:00 PM **Computational Evaluation of Coatings and Surface Treatments in Prevention of Fretting Fatigue:** *Xiawa Wu*<sup>1</sup>; Nathan Bolander<sup>1</sup>; Behrooz Jalalahmadi<sup>1</sup>; <sup>1</sup>Sentient Science
- 12:20 PM **Lunch Break**

## Applications II: Ferrous • Room: Colorado Ballroom II & III

- 2:00 PM **Development of Q&P Steels with Improved Performance based on Microstructure-based Finite Element Modeling Method:** *Kyoo Sil Choi*<sup>1</sup>; Xiaohua Hu<sup>1</sup>; Xin Sun<sup>1</sup>; Mark Taylor<sup>2</sup>; Emmanuel DeMoor<sup>2</sup>; John Speer<sup>2</sup>; David Matlock<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Colorado School of Mines
- 2:20 PM **ICME Towards Improved Understanding of Bainite in 100Cr6:** Wenwen Song<sup>1</sup>; Wolfgang Bleck<sup>1</sup>; *Ulrich Prah*<sup>1</sup>; <sup>1</sup>RWTH Aachen University
- 2:40 PM **ICME Approaches to Design Advanced Steels: Application to Transformation Induced Plasticity and Alumina Forming Stainless Steels:** *Raymundo Arroyave*<sup>1</sup>; Shengyen Li<sup>1</sup>; Taymaz Jozaghi<sup>1</sup>; Chung J. Wang<sup>1</sup>; Shujuan Wang<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; <sup>1</sup>Texas A & M University
- 3:00 PM **Steel – Ab initio: Quantum Mechanics Guided Design of New Fe-Based Materials:** *Wenwen Song*<sup>1</sup>; Ulrich Prah<sup>1</sup>; Wolfgang Bleck<sup>1</sup>; <sup>1</sup>RWTH Aachen University
- 3:20 PM **Break**
- 3:40 PM **Development of an ICME Framework for Steel Ingot Processing:** *Stephane Forsik*<sup>1</sup>; Jeffrey Yanke<sup>1</sup>; Richard Smith<sup>1</sup>; Mario Epler<sup>1</sup>; <sup>1</sup>Carpenter Technology Corporation
- 4:00 PM **Finite Element Modeling for Plymouth Tube Processing with Internal State Variables:** *Heecheen Cho*<sup>1</sup>; Youssef Hammi<sup>1</sup>; Mark Horstemeyer<sup>1</sup>; <sup>1</sup>Mississippi State University
- 4:20 PM **Ab-initio Calculation of Solute Effects on Austenite Grain Boundary Properties in Steel:** *Michael Hoerner*<sup>1</sup>; Mark Eberhart<sup>1</sup>; John Speer<sup>1</sup>; <sup>1</sup>Colorado School of Mines

## Modeling at Different Scales II • Room: Arkansas/Platte

- 2:00 PM **Multi-scale Simulation to Help Predict Morphology Generated by Reaction Induced Phase Separation:** *Dominic Wadkin-Snaith*<sup>1</sup>; Matthew Jackson<sup>1</sup>; <sup>1</sup>Cytec
- 2:20 PM **Virtual Testing of Polycrystalline Ni-based Superalloys: From Single Crystals to Design Allowables:** Aitor Cuadrado<sup>1</sup>; Bin Gan<sup>1</sup>; Javier Segurado<sup>2</sup>; Jon Mikel Molina-Aldareguía<sup>1</sup>; *Javier Llorca*<sup>2</sup>; <sup>1</sup>IMDEA Materials Institute; <sup>2</sup>Polytechnic University of Madrid & IMDEA Materials Institute
- 2:40 PM **Connecting Metallic Glass Mechanics with Its Deformation Physics via a Shear Transformation Zone Dynamics Model:** *Lin Li*<sup>1</sup>; <sup>1</sup>University of Alabama
- 3:00 PM **Multi-scale Modelling of Interfacial Energies on the Nanoscale: From Analytical to Quantum Mechanical:** *Wenwu Xu*<sup>1</sup>; Andrew Horsfield<sup>2</sup>; Peter Lee<sup>1</sup>; <sup>1</sup>The University of Manchester; <sup>2</sup>Imperial College London
- 3:20 PM **Break**
- 3:40 PM **A Multi-scale, Multi-physics Approach to Modelling of Fusion Welding in Titanium Alloys:** *Chinnapat Panwisawas*<sup>1</sup>; Yogesh Sovani<sup>1</sup>; Richard Turner<sup>1</sup>; Jeffery Brooks<sup>1</sup>; Hector Basoalto<sup>1</sup>; <sup>1</sup>University of Birmingham
- 4:00 PM **Multiscale Modeling using Probabilistic Description of Microstructure:** *Veera Sundararaghavan*<sup>1</sup>; John Allison<sup>1</sup>; Anna Trump<sup>1</sup>; Abhishek Kumar<sup>1</sup>; <sup>1</sup>University of Michigan
- 4:20 PM **Phase Field Simulation of Orowan Strengthening by Coherent Precipitate Plates in a Mg-Nd Alloy:** Hong Liu<sup>1</sup>; *Jian-Feng Nie*<sup>1</sup>; Yunzhi Wang<sup>2</sup>; <sup>1</sup>Monash University; <sup>2</sup>The Ohio State University

## ICME Models, Tools and Infrastructure I • Room: Rio Grande/Gunnison

- 2:00 PM **New Experimental Protocols for Mesoscale Studies of the Transformation of Retained Austenite to Martensite in Dual-Phase Steel:** *Ali Khosravani*<sup>1</sup>; Surya Kalidindi<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- 2:20 PM **Rapid Structure-Property Relationships Using Spherical Microindentation Stress-Strain Curves in Titanium Alloys:** *Jordan Weaver*<sup>1</sup>; Surya Kalidindi<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- 2:40 PM **Microtensile Characterization of Deformation and Failure of Fiber-reinforced Polymer Matrix Composites:** *Madhav Kolan*<sup>1</sup>; Jessica Krogstad<sup>1</sup>; Kevin Hemker<sup>1</sup>; Johns Hopkins University

- 3:00 PM High-Throughput Study of Phase Transformations and Microstructure Evolution using Diffusion Experiments:** Changdong Wei<sup>1</sup>; Qiaofu Zhang<sup>1</sup>; Siwei Cao<sup>1</sup>; *Ji-Cheng Zhao*<sup>1</sup>; <sup>1</sup>The Ohio State University
- 3:20 PM Break**
- 3:40 PM 3D Laboratory-based X-ray Diffraction Contrast Tomography of Polycrystalline Beta Titanium Alloys and Validation to EBSD and Synchrotron:** *Erik Lauridsen*<sup>1</sup>; Arno Merkle<sup>2</sup>; Peter Reischig<sup>3</sup>; Christian Holzner<sup>2</sup>; Michael Feser<sup>2</sup>; Kevin Fahey<sup>2</sup>; Henning Friis Poulsen<sup>2</sup>; Leah Lavery<sup>2</sup>; <sup>1</sup>Xnovo Technology ; <sup>2</sup>Carl Zeiss X-ray Microscopy, Inc.; <sup>3</sup>Xnovo Technology
- 4:00 PM Integrated Computational Model for Surface Strain Characterization in Stainless Steels and the Experimental Validation:** *Lili Zheng*<sup>1</sup>; Wei Wu<sup>2</sup>; Ke An<sup>2</sup>; Wei Yuan<sup>1</sup>; Harsha Badarinarayan<sup>1</sup>; <sup>1</sup>Hitachi America Ltd; <sup>2</sup>Oak Ridge National Lab
- 4:20 PM Investigating the Role of Microstructure in HCF and VHCF Regimes Using Ultrasonic Fatigue Methods:** *J. Wayne Jones*<sup>1</sup>; Jason Geathers<sup>1</sup>; Christopher Torbet<sup>2</sup>; Tresa M. Pollock<sup>2</sup>; Samantha Daly<sup>1</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>University of California Santa Barbara
- 4:40 PM Resonance Behavior Changes with Damage in Nickel-Based Superalloys:** *Brent Goodlet*<sup>1</sup>; Tresa Pollock<sup>1</sup>; <sup>1</sup>University of California, Santa Barbara

## Poster Session I • Room: Colorado Ballroom I • 5:00-6:30 PM

**Algorithms for Design Optimization of Hard Magnetic Alloys Using Experimental Data:** *George Dulikravich*<sup>1</sup>; Rajesh Jha<sup>1</sup>; Min Fan<sup>2</sup>; Justin Schwartz<sup>2</sup>; Carl Koch<sup>2</sup>; <sup>1</sup>Florida International University; <sup>2</sup>North Carolina State University

**An Integrated Finite Element Framework for the Hole Piercing to Hole Expansion Process of AA6111-T4 Sheets:** *Xiaohua Hu*<sup>1</sup>; Xin Sun<sup>1</sup>; Sergey Golovashchenko<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Ford Motor Company

**Application of Materials Modelling to Processing Simulation of Industrial Alloys:** *Zhanli Guo*<sup>1</sup>; <sup>1</sup>Sente Software Ltd.

**CALPHAD-based and Experimental Investigations of Microstructures in Austenitic Heat-resistant Cast Steels for Exhaust Component Applications:** *Yinhui Zhang*<sup>1</sup>; Mei Li<sup>2</sup>; Larry Godlewski<sup>2</sup>; Jacob Zindel<sup>2</sup>; Qiang Feng<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Ford Motor Company

**Coating on Performance:** *Dieter Heumannskaemper*<sup>1</sup>; <sup>1</sup>Morgan Advanced Materials

**Degradation of Crucible Properties and Impact on Energy Consumption During Operation:** Dieter Heumannskaemper<sup>1</sup>; *Mirco Pavoni*<sup>1</sup>; <sup>1</sup>Morgan Advanced Materials

**Design of Co-free Cemented Carbides:** *Martin Walbrüh*<sup>1</sup>; John Ågren<sup>1</sup>; Annika Borgenstam<sup>1</sup>; <sup>1</sup>KTH - Royal Institute of Technology

**Effect of Die Design Parameters on the Stresses Generated during the Closed Die Forging Process:** *Santosh Kumar*<sup>1</sup>; Atul Patil<sup>1</sup>; Shreyas Kirwai<sup>1</sup>; <sup>1</sup>Bharat Forge Limited

**Effect of Lime Causticization on Silica, Calcium, Oxalate and Organic Carbon Levels in Bayer Process Washer Overflow Liquor:** *Max Wellington*<sup>1</sup>; <sup>1</sup>Northern Caribbean University

**Effect of Shape Oscillations on the Stability of a Particle Laden Bubble during Rising:** *Prithvi Yesudas*<sup>1</sup>; Sabita Sarkar<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Madras

**Efficient Degassing for Aluminium Melting:** Dieter Heumannskaemper<sup>1</sup>; Mirco Pavoni<sup>1</sup>; *Arjoon Vohra*<sup>1</sup>; <sup>1</sup>Morgan Advanced Materials

**Experimental and Numerical Determination of the Fracture Energy of Carbon Fiber Reinforced Phenolic Resin-based Plastics Composites:** *Khurram Iqbal*<sup>1</sup>; <sup>1</sup>Dalian University of Technology

**Experimental Verification for Solid Fraction Measurement in Semi-solid Silver Metal Processing in Comparisons with Theoretical Thermodynamics Modeling:** *Pun Wiro*<sup>1</sup>; Boonrat Lohwongwattana<sup>1</sup>; Ekasit Nisaratanaporn<sup>1</sup>; <sup>1</sup>Chulalongkorn University

**Exploring the Performance-Property-Structure Solution Space in Friction Stir Welding:** *Chung Hyun Goh*<sup>1</sup>; Adam Dachowicz<sup>1</sup>; Janet Allen<sup>1</sup>; Farrokh Mistree<sup>1</sup>; <sup>1</sup>University of Oklahoma

**Force Modelling for Temperature Field determination During High Speed End-Milling of Superalloys:** *Sunday Ojolo*<sup>1</sup>; Oluwole Adesina<sup>2</sup>; Gbeminiyi Sobamowo<sup>1</sup>; <sup>1</sup>University of Lagos; <sup>2</sup>Yaba Colege of Technology

**High Entropy Nickel Superalloys Designed via the CALPHAD Method:** *Joseph Licavoli*<sup>1</sup>; Paul Jablonski<sup>1</sup>; Jeff Hawk<sup>1</sup>; <sup>1</sup>Department of Energy

**Hot Deformation Behavior and 3D Processing Maps of Extruded AZ61 Magnesium Alloy:** *Juqiang Li*<sup>1</sup>; <sup>1</sup>Shanghai Jiao Tong University

**Performance Enhancement of SiC Heating Elements by Virtue of Simulation:** *Yongwoo Kwon*<sup>1</sup>; *Youngjae Cho*<sup>1</sup>; *Jonghuck Lee*<sup>1</sup>; *Seung-Yong Lee*<sup>2</sup>; *Young-Min Kong*<sup>3</sup>; <sup>1</sup>Hongik University; <sup>2</sup>Korea Institute of Science and Technology; <sup>3</sup>University of Ulsan

**Phase-field Modeling of Morphological Evolution of a Charged Particle:** *Dong-Uk Kim*<sup>1</sup>; *Hee-Chul Yang*<sup>1</sup>; *Pil-Ryung Cha*<sup>1</sup>; <sup>1</sup>Kookmin University

**Prediction of Particle Recovery and Wall Stress due to Submerged Swirling Gas Jet-liquid Interaction:** *Vishnu Mantripragada*<sup>1</sup>; *Sabita Sarkar*<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Madras

**Structure-Property Modeling Tools for Triplex Mo-Si-B Alloys:** *Kyle Brindley*<sup>1</sup>; *Richard Neu*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

**Synthesis and Characterisation of Al Doped ZnO Nanoparticles:** *Chitrashi Mahajan*<sup>1</sup>; <sup>1</sup>NIT

**The Finite Element Analysis to Improving the Effect of Thick Slab Continuous Casting Bulging:** *Weihua Wang*<sup>1</sup>; <sup>1</sup>Shougang Research Institute of Technology

**Towards Plug & Play in ICME – Pathways Towards Communication Standards and Interface Specifications:** *Georg Schmitz*<sup>1</sup>; <sup>1</sup>Access e.V.

**Tuesday, June 2, 2015**

**Applications III: Composites and Non-Ferrous • Room: Colorado Ballroom II & III**

**8:00 AM Exploiting Interfaces in Multi-scale Topology Optimization for ICME:** *Natasha Vermaak*<sup>1</sup>; <sup>1</sup>Lehigh University

**8:20 AM Integrated Computational Methods for Composites Materials (ICM2): Lessons Learned From Integration Planning and Feasibility Demonstrations:** *Lara Liou*<sup>1</sup>; <sup>1</sup>GE Aviation

**8:40 AM Use of a Computational Method to Develop a New Composite Matrix Chemistry with Improved Performance:** *Stephen Christensen*<sup>1</sup>; <sup>1</sup>Boeing Research & Technology

**9:00 AM Manufacturing Process Induced Effects in Mechanical Behavior of Carbon FRPCs:** *Marianna Maiaru*<sup>1</sup>; *Royan D'Mello*<sup>1</sup>; *Pavana Prabhakar*<sup>2</sup>; *Folusho Oyerokun*<sup>3</sup>; *Matthew Hockemeyer*<sup>4</sup>; *Li Zheng*<sup>4</sup>; *Anthony Waas*<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor; <sup>2</sup>University of Texas, El Paso; <sup>3</sup>GE Aviation; <sup>4</sup>GE Global Research

**9:20 AM Capturing Size Effects in Composites Using Progressive Failure Stochastic Simulation:** *Seyed Hamid Reza Sanei*<sup>1</sup>; *Ray Fertig*<sup>1</sup>; <sup>1</sup>University of Wyoming

**9:40 AM Break**

**10:00 AM Severe Plastic Deformation of Ti for Biomedical Applications: From Processing to Performance:** *Hyoung Seop Kim*<sup>1</sup>; *Dong-Hyun Ahn*<sup>1</sup>; <sup>1</sup>POSTECH

**10:20 AM Application of Multi-Scale Fatigue Models in Lightweight Metal Castings:** *Qigui Wang*<sup>1</sup>; <sup>1</sup>General Motors

**10:40 AM Modelling Stress-assisted Grain Oxidation Ahead of a Crack in a Nickel-based Superalloy:** *Chizhou Fang*<sup>1</sup>; *Hector Basoalto*<sup>1</sup>; *Hangyue Li*<sup>1</sup>; *Steve Williams*<sup>2</sup>; *Hugh Evans*<sup>1</sup>; <sup>1</sup>University of Birmingham; <sup>2</sup>Rolls-Royce plc

**11:00 AM Polymers on the Edge of Metallic Conductivity and Their Aerospace Applications:** *Ekaterina Badaeva*<sup>1</sup>; *Patrick Kinfen*<sup>1</sup>; *Ofer Alves*<sup>1</sup>; <sup>1</sup>Boeing

**11:20 AM Yield Strength Model for Undercooled Aluminium Alloys Based on Calorimetric In-situ Quenching Experiments:** *Michael Reich*<sup>1</sup>; *Philipp Schumacher*<sup>1</sup>; *Benjamin Milkereit*<sup>1</sup>; *Olaf Kessler*<sup>1</sup>; <sup>1</sup>University of Rostock

**11:40 AM A Combined Experimental and Molecular Dynamics Investigation of Dislocation-based Hardening Mechanisms in Co-Ni Multilayers with a Bimodal Grain Size Distribution:** *Matthew Daly*<sup>1</sup>; *Chandra Veer Singh*<sup>1</sup>; *Glenn Hibbard*<sup>1</sup>; <sup>1</sup>University of Toronto

**12:00 PM Lunch Break**

**ICME Implementation and Case Studies • Room: Arkansas/Platte**

**8:00 AM Developing Refractory High-Entropy Alloys: Computation-Guided Experiments:** *Michael Gao*<sup>1</sup>; *J.W. Qiao*<sup>2</sup>; *B. Zhang*<sup>3</sup>; *H.W. Yao*<sup>2</sup>; *S.M. Guo*<sup>3</sup>; *S.Z. Yang*<sup>4</sup>; *C.S. Carney*<sup>1</sup>; *P.J. Jablonski*<sup>1</sup>; *J.A. Hawk*<sup>1</sup>; *D.E. Alman*<sup>1</sup>; <sup>1</sup>National Energy Technology Lab; <sup>2</sup>Taiyuan Institute of Technology; <sup>3</sup>Louisiana State University; <sup>4</sup>Southern University and A&M College

**8:20 AM ICME Based Accelerated Materials Innovation:** *Jiadong Gong*<sup>1</sup>; *David Snyder*<sup>1</sup>; *Jason Sebastian*<sup>1</sup>; *Greg Olson*<sup>1</sup>; <sup>1</sup>QuesTek Innovations



- 8:40 AM** **A Computational Framework for Designing g/g' Co-based Superalloys:** *Shengyen Li<sup>1</sup>; Eric Lass<sup>1</sup>; Daniel Wheeler<sup>1</sup>; Ursula Kattner<sup>1</sup>; Carelyn Campbell<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology*
- 9:00 AM** **Development of an ICME Approach for Aluminum Alloy Corrosion:** *Kenneth Smith<sup>1</sup>; Mark Jaworowski<sup>1</sup>; Rajiv Ranjan<sup>1</sup>; George Zafiris<sup>1</sup>; <sup>1</sup>United Technologies Research Center*
- 9:20 AM** **ICME and the Industrial Enterprise: Early Successes, Implementation, and Simplification:** *Katherine Stevens<sup>1</sup>; Jeffrey Williams<sup>1</sup>; Sanjay Sondhi<sup>2</sup>; <sup>1</sup>GE Aviation; <sup>2</sup>GE Global Research*
- 9:40 AM** **Break**
- 10:00 AM** **Adaptive Electronic Materials by Design:** *James Booth<sup>1</sup>; Nathan Orloff<sup>1</sup>; Darrell Schlom<sup>2</sup>; Craig Fennie<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>Cornell University*
- 10:20 AM** **Utilizing ICME Models to More Effectively Predict Process-Structure-Property Relationships for Better Property Optimization and Design in Aerospace Alloys:** *Ashley Goulding<sup>1</sup>; Richard Neu<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology*
- 10:40 AM** **Utilizing the Bond Bundle for Material Design:** *Jonathan Miorelli<sup>1</sup>; <sup>1</sup>Colorado School of Mines*
- 11:00 AM** **ICME Support for Jumbo Vertical Bloom Continuous Caster:** *Patrick Anderson<sup>1</sup>; Krich Sawamiphakdi<sup>1</sup>; Dongbu Cao<sup>1</sup>; Christopher Eastman<sup>1</sup>; <sup>1</sup>TimkenSteel Corporation*
- 11:20 AM** **Lunch Break**

## ICME Models, Tools and Infrastructure II • Room: Rio Grande/Gunnison

- 8:00 AM** **Coupling Phase-field Modeling and Real Time Synchrotron X-ray Observation to Analyze the Influence of Cooling Rate on the Dendritic Morphology of Mg-Gd Alloys during Solidification:** *Yongbiao Wang<sup>1</sup>; Liming Peng<sup>1</sup>; Longqing Chen<sup>2</sup>; <sup>1</sup>Shanghai Jiaotong University; <sup>2</sup>Pennsylvania State University*
- 8:20 AM** **Application of Machine Learning Techniques for Inverse Prediction in Manufacturing Process Chains:** *Sapan Shah<sup>1</sup>; Sreedhar Reddy<sup>1</sup>; Avadhut Sardeshmukh<sup>1</sup>; BP Gautham<sup>1</sup>; Gautam Shroff<sup>1</sup>; Ashwin Srinivasan<sup>2</sup>; <sup>1</sup>TRDDC, Tata Consultancy Services; <sup>2</sup>IIT, Delhi*
- 8:40 AM** **Capturing and Transforming Phase-Based Materials Data: The Materials Data Curator:** *Carelyn Campbell<sup>1</sup>; Alden Dima<sup>1</sup>; Sharief Youssef<sup>1</sup>; Philippe Dessauw<sup>1</sup>; Guillaume Sousa Amaral<sup>1</sup>; Mary Brady<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology*
- 9:00 AM** **Facilitating the Selection and Creation of Interatomic Potentials (Force Fields) with Robust Modeling Tools and a New Data Infrastructure:** *Zachary Trautt<sup>1</sup>; Chandler Becker<sup>1</sup>; Lucas Hale<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology*
- 9:20 AM** **nanoHUB as a Platform for Implementing ICME Simulations in Research and Education:** *Tanya Faltens<sup>1</sup>; Alejandro Strachan<sup>2</sup>; Gerhard Klimeck<sup>2</sup>; <sup>1</sup>Purdue/ NCN; <sup>2</sup>Purdue University*
- 9:40 AM** **Break**
- 10:00 AM** **A Review of Materials Data Infrastructure Projects:** *Scott Henry<sup>1</sup>; Larry Berardinis<sup>1</sup>; <sup>1</sup>ASM International*
- 10:20 AM** **Atomistic Simulations of Polymers in the Cloud: Resources for Research and Education:** *Alejandro Strachan<sup>1</sup>; Benjamin Haley<sup>1</sup>; Chunyu Li<sup>1</sup>; <sup>1</sup>Purdue University*
- 10:40 AM** **An Integrated Collaborative Environment for Materials Research:** *Mark Benedict<sup>1</sup>; Matthew Jacobsen<sup>1</sup>; Bryon Foster<sup>1</sup>; Charles Ward<sup>1</sup>; <sup>1</sup>USAF/AFRL*
- 11:00 AM** **Computational Characterization of Network Structure and Nanovoid Growth of Thermoset Polymers:** *Chunyu Li<sup>1</sup>; Alejandro Strachan<sup>1</sup>; <sup>1</sup>Purdue University*
- 11:20 AM** **Uncertainty Quantification of Quantitative Structure-property Relationship Models of Composites:** *Paul Patrone<sup>1</sup>; Andrew Dienstfrey<sup>2</sup>; Stephen Christensen<sup>3</sup>; Samuel Tucker<sup>3</sup>; Andrea Browning<sup>3</sup>; <sup>1</sup>IMA; <sup>2</sup>NIST; <sup>3</sup>Boeing*
- 11:40 AM** **PyMKS: A Tool for Modeling Microstructure/Response Relationships in Python:** *Daniel Wheeler<sup>1</sup>; David Brough<sup>2</sup>; Tony Fast<sup>2</sup>; Surya Kalidindi<sup>2</sup>; <sup>1</sup>NIST; <sup>2</sup>Georgia Institute of Technology*
- 12:00 PM** **Lunch Break**

## Plenary Session II • Room: Colorado Ballroom II & III

- 2:00 PM** **Invited  
Integrated Computational Materials Engineering (ICME) of Generation Three Advanced High Strength Steels:** *Louis Hector Jr<sup>1</sup>; <sup>1</sup>General Motors*

- 2:20 PM** **Invited**  
**An ICME Approach to Nanostructure Design via Non-conventional Phase Transformation Pathways in Multi-phase Alloys:** Rongpei Shi<sup>1</sup>; Dong Wang<sup>2</sup>; Yufeng Zheng<sup>1</sup>; Hamish Fraser<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Xi'an Jiao Tong University
- 2:40 PM** **Invited**  
**Integrated Computational Materials Engineering Approach to Automotive Lightweighting:** Kaan Inal<sup>1</sup>; Raja Mishra<sup>2</sup>; <sup>1</sup>University of Waterloo; <sup>2</sup>General Motors R&D
- 3:00 PM** **Invited**  
**Importance of Controlling Microstructure Heterogeneity When Designing Steel:** Kohsaku Ushioda<sup>1</sup>; Hideaki Sawada<sup>1</sup>; Masaaki Sugiyama<sup>1</sup>; <sup>1</sup>Nippon Steel & Sumitomo Metal Corp.
- 3:20 PM** **Invited**  
**ICME for Process Scale-up: Importance of Vertical and Horizontal Integration of Models:** Gerald Tennyson<sup>1</sup>; Rishabh Shukla<sup>1</sup>; Saurabh Mangal<sup>1</sup>; Savya Sachi<sup>1</sup>; Amarendra Singh<sup>1</sup>; <sup>1</sup>Tata Consultancy Services
- 3:40 PM** **Break**
- 4:00 PM** **ICME Tools Showcase**

## Poster Session II • Room: Colorado Ballroom I • 5:00-6:30 PM

**A Curve Swarm Algorithm for Global Search of State Transition Paths:** Lijuan He<sup>1</sup>; Yan Wang<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

**A Quantized Crystal Plasticity Model for Nanocrystalline Metals: Connecting Atomistic Simulations and Physical Experiments:** Lin Li<sup>1</sup>; <sup>1</sup>University of Alabama

**An Interface to Quantum ESPRESSO:** Linu Malakkal<sup>1</sup>; Barbara Szpunar<sup>1</sup>; Juan Zuniga<sup>1</sup>; Ravi Siripurapu<sup>1</sup>; Jerzy Szpunar<sup>1</sup>; <sup>1</sup>University of Saskatchewan

**Analysis of Published Cast Iron Experimental Data.:** Siddhartha Biswas<sup>1</sup>; Charles Monroe<sup>1</sup>; Thomas Prucha<sup>2</sup>; <sup>1</sup>University of Alabama at Birmingham; <sup>2</sup>American Foundry Society

**Applying Inverse Algorithm for In-Situ Resonance Inspection:** Kevin Lai<sup>1</sup>; Wei Xu<sup>1</sup>; Xin Sun<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

**Atomistic Modeling of Epoxy CNT Nanocomposites:** Veera Sundararaghavan<sup>1</sup>; Nicholas Fasanella<sup>1</sup>; <sup>1</sup>University of Michigan

**Benchmarking Multi-scale Models through Micro-mechanical Testing and Characterization of Ni-base Superalloys:** David Eastman<sup>1</sup>; Zafir Alam<sup>1</sup>; Jessica Krogstad<sup>2</sup>; George Weber<sup>1</sup>; Somnath Ghosh<sup>1</sup>; William Lenhe<sup>3</sup>; Tresa Pollock<sup>3</sup>; Paul Shade<sup>4</sup>; Michael Uchic<sup>4</sup>; Kevin Hemker<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>University of Illinois, Urbana-Champaign; <sup>3</sup>University of California Santa Barbara; <sup>4</sup>Air Force Research Laboratory

**Bondalyzer: A Tool for the Discovery of Charge Density Property Relationships:** Tim Wilson<sup>1</sup>; <sup>1</sup>Colorado School of Mines

**Building the Materials Databases and Exploring the Potential Application for Materials Design:** Haiqing Yin<sup>1</sup>; Ruijie Zhang<sup>1</sup>; Guoquan Liu<sup>1</sup>; Xuanhui Qu<sup>1</sup>; Jianxin Xie<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

**Coarse-Graining Simulations of the Correlation between Free Volume Evolution and Plastic Deformation of Highly Cross-Linked DGEBA Polymer:** Amin Aramoon<sup>1</sup>; Stephen Barr<sup>2</sup>; Timothy Brietzman<sup>2</sup>; Christopher Woodward<sup>2</sup>; Jaafar El-Awady<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>Air Force Research Laboratory

**Dimension Tolerance Analysis of Aluminum Casting Components:** Quan Zhibin<sup>1</sup>; Zhiqiang Gao<sup>1</sup>; Qigui Wang<sup>2</sup>; <sup>1</sup>Southeast University, China; <sup>2</sup>General Motors Corporation

**Discrete Dislocation Dynamics Simulation of the Effect of Tension-Twins on the Plastic Deformation of Magnesium Crystals:** Haidong Fan<sup>1</sup>; Sylvie Aubry<sup>2</sup>; A. Arsenlis<sup>2</sup>; Jaafar El-Awady<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>Lawrence Livermore National Laboratory

**Energy Landscape of  $\{111\}$ -Grain Boundaries: The Space of Boundary-Plane Orientations:** Arash Dehghan Banadaki<sup>1</sup>; Srikanth Patala<sup>1</sup>; <sup>1</sup>North Carolina State University

**MedeA® - an Atomistic Simulation Environment for ICME:** Paul Saxe<sup>1</sup>; Clive Freeman<sup>1</sup>; Erich Wimmer<sup>2</sup>; <sup>1</sup>Materials Design, Inc.; <sup>2</sup>Materials Design, SARL

**Mesoscale Modeling of 3-d Voids Evolution in Large Ingot during Multi-hit Deformation:** Zhenshan Cui<sup>1</sup>; Chao Feng<sup>1</sup>; Xiaoqing Shang<sup>1</sup>; Xinjia Li<sup>1</sup>; <sup>1</sup>Shanghai Jiao Tong University

**Micromechanical Approach for R-value Prediction of Dual-phase Steel:** *Jinjin Ha*<sup>1</sup>; Ji Hoon Kim<sup>2</sup>; Myoung-gyu Lee<sup>3</sup>; Frédéric Barlat<sup>1</sup>; <sup>1</sup>Pohang University of Science and Technology (POSTECH); <sup>2</sup>Busan National University; <sup>3</sup>Korea University

**Microstructure Design in LENS Manufactured Components:** *Jacob Smith*<sup>1</sup>; Jian Cao<sup>1</sup>; Wing Kam Liu<sup>1</sup>; <sup>1</sup>Northwestern University

**Modeling and Experimental Verification of Fragmentation in Metal Alloys:** *Doyle Dickey*<sup>1</sup>; Mark Horstemeyer<sup>1</sup>; <sup>1</sup>Mississippi State University

**Modelling the Microstructure of Polycrystalline Austenite-martensite Steels:** *Alireza Rahnama*<sup>1</sup>; Rongshan Qin<sup>1</sup>; <sup>1</sup>Imperial College

**Multiscale Modelling Platform: Smart Design of Nano-enabled Products in Green Technologies:** J.P. Krugers<sup>1</sup>; D. Roosen-Melsen<sup>1</sup>; E. Coenen<sup>1</sup>; *Georg Schmitz*<sup>2</sup>; M. van den Brand<sup>3</sup>; T. Verhoeff<sup>3</sup>; O. Babur<sup>3</sup>; B. Patzák<sup>4</sup>; V. Smilauer<sup>4</sup>; G. Pacquaut<sup>4</sup>; M. Apel<sup>2</sup>; R. Altenfeld<sup>2</sup>; J. Olkkonen<sup>5</sup>; P. Myöhänen<sup>5</sup>; A.M. Lankhorst<sup>6</sup>; L. Thielen<sup>6</sup>; W.D. van Driel<sup>7</sup>; V. Hildenbrand<sup>7</sup>; J.M. Delgado Sanchez<sup>8</sup>; E. Sanchez Cortezon<sup>8</sup>; <sup>1</sup>TNO; <sup>2</sup>Access RWTH Aachen; <sup>3</sup>TU Eindhoven; <sup>4</sup>Czech Technical University; <sup>5</sup>VTT; <sup>6</sup>Celsian; <sup>7</sup>Philips; <sup>8</sup>Abengoa

**Numerical Investigation of Microstructural Features on the Damage Behavior of Ceramic Matrix Composites:** *Pascal Meyer*<sup>1</sup>; Anthony Waas<sup>1</sup>; <sup>1</sup>University of Michigan

**Optimization of a Platinum-nickel Surface by DFT Calculations:** Emiliano Diez Tortorella<sup>1</sup>; Sandra Ulacco<sup>1</sup>; *Sandra Simonetti*<sup>2</sup>; <sup>1</sup>UTN; <sup>2</sup>UTN-UNS-CONICET

**Performance Evaluation, Algorithm Optimization and Sensitivity Analysis of the Spectral Full-Field Deformation Modeling of Polycrystalline Materials:** *Tugce Ozturk*<sup>1</sup>; Clayton Stein<sup>1</sup>; Reeru Pokharel<sup>2</sup>; Thom Popovici<sup>1</sup>; Franz Franchetti<sup>1</sup>; Robert Suter<sup>1</sup>; Anthony Rollett<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Los Alamos National Laboratory

**Probabilistic Occurrence of Weakest Link Microstructural Features in Two-Phase Titanium:** *Joseph Tucker*<sup>1</sup>; Tyler Weihing<sup>2</sup>; Michael Groeber<sup>3</sup>; Adam Pilchak<sup>3</sup>; <sup>1</sup>UES, Inc.; <sup>2</sup>Southwestern Ohio Council for Higher Education; <sup>3</sup>Air Force Research Laboratory

**Simulation of Microstructural Evolution of Three-dimensional Synthetic Microstructures during Deformation for Two-phase Titanium Alloys:** *Sudipto Mandal*<sup>1</sup>; Anthony Rollett<sup>1</sup>; Shanoob Balachandran<sup>2</sup>; Dipankar Banerjee<sup>2</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Indian Institute of Science Bangalore

**Study of the Influence of Heat Source Parameters and Build Profile on the Melt pool Dynamics in Additive Manufacturing:** *Narendran Raghavan*<sup>1</sup>; Sreekanth Pannala<sup>2</sup>; Srdjan Simunovic<sup>2</sup>; Neil Carlson<sup>3</sup>; Sudarsanam Babu<sup>1</sup>; John Turner<sup>2</sup>; <sup>1</sup>University of Tennessee Knoxville; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>Los Alamos National Laboratory

## Wednesday, June 3, 2015

### Plenary Session III • Room: Colorado Ballroom II & III

8:00 AM	<b>Invited</b> <b>Integrated Computational Materials Engineering Needs for Aerospace:</b> <i>James Cotton</i> <sup>1</sup> ; RJ Glamm <sup>1</sup> ; DM Rosenblatt <sup>1</sup> ; E Pripstein <sup>1</sup> ; S Christensen <sup>1</sup> ; <sup>1</sup> Boeing
8:20 AM	<b>Invited</b> <b>Data Infrastructure Developed for PW-8: Nickel Base Superalloy Residual Stress Foundational Engineering Problem:</b> <i>Terry Wong</i> <sup>1</sup> ; Vasisht Venkatesh <sup>2</sup> ; Todd J Turner <sup>3</sup> ; <sup>1</sup> Aerojet Rocketdyne; <sup>2</sup> Pratt & Whitney; <sup>3</sup> Air Force Research Laboratory
8:40 AM	<b>Invited</b> <b>Modeling and Simulation of Directional Solidification of Ni-Based Superalloy Turbine Blades Casting Assisted by Liquid Metal Cooling:</b> Qingyan Xu <sup>1</sup> ; Ning Tang <sup>1</sup> ; <i>Baicheng Liu</i> <sup>1</sup> ; <sup>1</sup> Tsinghua University
9:00 AM	<b>Invited</b> <b>From Integrated Computational Materials Engineering to Integrated Computational Structural Engineering:</b> <i>Rollie Dutton</i> <sup>1</sup> ; Pam Kobryn <sup>1</sup> ; Dale Ball <sup>2</sup> ; James Castle <sup>3</sup> ; Mark James <sup>4</sup> ; Parviz Yavari <sup>5</sup> ; <sup>1</sup> Air Force Research Laboratory; <sup>2</sup> Lockheed Martin Aeronautics Company; <sup>3</sup> Boeing Research & Technology; <sup>4</sup> Alcoa; <sup>5</sup> Northrup Grumman Corporation
9:20 AM	<b>Invited</b> <b>Preparing for the Future of Computing: Bridging Scales within the Exascale Materials Co-design Center*:</b> <i>James Belak</i> <sup>1</sup> ; <sup>1</sup> Lawrence Livermore National Laboratory
9:40 AM	<b>Question and Answer Period</b>
10:00 AM	<b>Break</b>

## Process and Performance Modeling II • Room: Colorado Ballroom II & III

- 10:20 AM** **A General Simulation Technology for Forging with Considering the Evolution of Voids, Grains and Cracks:** Xinjia Li<sup>1</sup>; Xiaoqing Shang<sup>1</sup>; *Zhenshan Cui*<sup>1</sup>; Chao Feng<sup>1</sup>; Dingqian Dong<sup>1</sup>; Shanghai Jiao Tong University
- 10:40 AM** **A Method for Determining the Set Points of the Ladle, Tundish and Caster for Manufacturing a High Strength Steel Slab:** *Rishabh Shukla*<sup>1</sup>; Ravikiran Anapagaddi<sup>1</sup>; Janet Allen<sup>2</sup>; Jitesh Panchal<sup>3</sup>; Farrokh Mistree<sup>2</sup>; Amarendra Singh<sup>1</sup>; <sup>1</sup>Tata Research, Development and Design Center; <sup>2</sup>University of Oklahoma; <sup>3</sup>Purdue University
- 11:00 AM** **ICME for the Integrated Design of an Automotive Gear Considering Uncertainty:** *BP Gautham*<sup>1</sup>; Nagesh Kulkarni<sup>1</sup>; Pramod Zagade<sup>1</sup>; Janet Allen<sup>2</sup>; Farrokh Mistree<sup>2</sup>; Jitesh Panchal<sup>3</sup>; <sup>1</sup>Tata Research, Development and Design Center; <sup>2</sup>University of Oklahoma; <sup>3</sup>Purdue University
- 11:20 AM** **Gamma Prime Evolution during Processing and Heat Treatment of the Nickel-Based Superalloy IN738LC.:** *Magnus Anderson*<sup>1</sup>; Andrew Rowe<sup>2</sup>; Jonathon Wells<sup>3</sup>; Hector Basoalto<sup>1</sup>; <sup>1</sup>University of Birmingham; <sup>2</sup>RWE npower; <sup>3</sup>Siemens Industrial Turbomachinery Limited
- 11:40 AM** **Investigating the Influence of Microstructural Features on Strength and Ductility of Beta Annealed Ti-6Al-4V:** *Matt Kasemer*<sup>1</sup>; Euan Wielewski<sup>1</sup>; Romain Quey<sup>2</sup>; Paul Dawson<sup>1</sup>; <sup>1</sup>Cornell University; <sup>2</sup>Ecole des Mines de Saint-Étienne
- 12:00 PM** **Multiphysics Modeling and Simulation of Electromagnetic Pulse Welding:** *Wei Xu*<sup>1</sup>; Alexander Mamutov<sup>2</sup>; Dangxin Wu<sup>1</sup>; Xin Sun<sup>1</sup>; John Bonnen<sup>2</sup>; Quochung Le<sup>2</sup>; Sergey Golovashchenko<sup>3</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Ford Research & Advanced Engineering; <sup>3</sup>Oakland University
- 12:20 PM** **Through-process Modeling for Alloy Design and Process Optimization for Cold Spray Processing:** *Danielle Belsito*<sup>1</sup>; Baillie McNally<sup>1</sup>; Victor Champagne<sup>2</sup>; Richard Sisson<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute; <sup>2</sup>U.S. Army Research Laboratory
- 12:40 PM** Lunch Break

## Modeling at Different Scales III • Room: Arkansas/Platte

- 10:20 AM** **Calibrated Localization Relationships for Polycrystalline Aggregates by using Materials Knowledge System:** *Yuksel Yabansu*<sup>1</sup>; Surya Kalidindi<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- 10:40 AM** **An Efficient Hybrid 2D/3D Discrete Dislocation Dynamics Simulation for Engineering Dislocations Structures in Thin Films:** *Siavash Sarrafan*<sup>1</sup>; Ray Fertig<sup>1</sup>; <sup>1</sup>University of Wyoming
- 11:00 AM** **Computational Modeling and Experimental Characterization of Martensitic Transformations in NiCoAl for Self-Sensing Materials:** *Terry Wallace*<sup>1</sup>; Vesselin Yamakov<sup>2</sup>; Jacob Hochhalter<sup>1</sup>; William Leser<sup>1</sup>; James Warner<sup>1</sup>; John Newman<sup>1</sup>; Ganga Purja Pun<sup>3</sup>; Yuri Mishin<sup>3</sup>; <sup>1</sup>NASA Langley Research Center; <sup>2</sup>National Institute of Aerospace; <sup>3</sup>George Mason University
- 11:20 AM** Break
- 11:40 AM** **A Progressive Damage Model for Ceramic Matrix Composites with Processing-Induced Residual Stress:** *Lucas Hansen*<sup>1</sup>; Anthony Waas<sup>1</sup>; <sup>1</sup>University of Michigan
- 12:00 PM** **Effect of Interface Dislocation Recovery on the Strain-hardening Rate of the Nanolayered Metallic Composites: An Atomistically Informed Interface Dislocation Dynamics Investigation:** *Shuai Shao*<sup>1</sup>; Jian Wang<sup>1</sup>; Caizhi Zhou<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Missouri University of Science and Technology
- 12:20 PM** **From Melt Pool to Strength - Application of ICME Methods for the Development of Rapid Manufacturing Technologies:** *Tobias Maiwald-Immer*<sup>1</sup>; Thomas Goehler<sup>1</sup>; Andreas Fischersworing-Bunk<sup>1</sup>; <sup>1</sup>MTU Aero Engines AG
- 12:40 PM** Lunch Break

## ICME Models, Tools and Infrastructure III • Room: Rio Grande/Gunnison

- 10:20 AM** **CALPHAD Modeling and Microstructure Investigation of Mg-Al-Sn-Ca/Sr Systems:** Weihua Sun<sup>1</sup>; *Alan Luo*<sup>1</sup>; <sup>1</sup>The Ohio State University
- 10:40 AM** **The Inverse Phase Stability as a Constraint Satisfaction Problem:** *Richard Malak*<sup>1</sup>; Edgar Galvan<sup>1</sup>; Sean Gibbons<sup>1</sup>; Raymundo Arroyave<sup>1</sup>; <sup>1</sup>Texas A & M University
- 11:00 AM** **Modeling the Formation of Eutectic Castings:** *Oriane Senninger*<sup>1</sup>; Peter Voorhees<sup>1</sup>; <sup>1</sup>Northwestern University
- 11:20 AM** Break
- 11:40 AM** **Predictive Simulation of Diffusion in Ni-based Alloys using Pair Interaction Model Based Kinetic Monte Carlo Method:** *Dominic Alfonso*<sup>1</sup>; De Nyago Tafen<sup>2</sup>; <sup>1</sup>National Energy Technology Laboratory - DOE; <sup>2</sup>National Energy Technology Laboratory / URS Corporation

**12:00 PM** **Thermodynamic and Diffusion Mobility Modeling of the Aluminum-Hydrogen-Nickel-Oxygen System Augmented by First-principles Techniques:** *Austin Ross*<sup>1</sup>; Xuan Liu<sup>1</sup>; Greta Lindwall<sup>1</sup>; Huazhi Fang<sup>1</sup>; Zi-Kui Liu<sup>1</sup>; <sup>1</sup>Pennsylvania State University

**12:20 PM** **Effect of Dislocation Density and Crystal Size on Surface Roughness Evolution under Cyclic Loading in FCC Metals from Discrete Dislocation Dynamics Simulations:** *Ahmed Hussein*<sup>1</sup>; Jaafar El-Awady<sup>1</sup>; <sup>1</sup>Johns Hopkins University

**12:40 PM** **Lunch Break**

**Other • Room: Colorado Ballroom II & III**

**2:00 PM** **An Integrated Surrogate Modeling Approach for Materials and Process Design:** *Melanie Senn*<sup>1</sup>; <sup>1</sup>Fraunhofer IWM

**2:20 PM** **Uncertainty Management in the Integrated Realization of Materials and Components:** *Janet Allen*<sup>1</sup>; Jitesh Panchal<sup>2</sup>; Farrokh Mistree<sup>1</sup>; Amarendra Singh<sup>3</sup>; BP Gautham<sup>3</sup>; <sup>1</sup>University of Oklahoma; <sup>2</sup>Purdue University; <sup>3</sup>Tata Research, Development and Design Center

**2:40 PM** **Analysis of Strengthening in AA6111 during the Early Stages of Aging:** *Alban de Vaucorbeil*<sup>1</sup>; Ross Marceau<sup>2</sup>; Gang Sha<sup>3</sup>; Simon Ringer<sup>3</sup>; Warren Poole<sup>1</sup>; <sup>1</sup>University of British Columbia; <sup>2</sup>Deakin University; <sup>3</sup>University of Sydney

**3:00 PM** **The Materials Commons: A Novel Information Repository and Collaboration Platform for the Materials Community:** *Brian Puchala*<sup>1</sup>; Glenn Tarcea<sup>1</sup>; Emmanuelle Marquis<sup>1</sup>; Sravya Tamma<sup>1</sup>; John Allison<sup>1</sup>; <sup>1</sup>The University of Michigan

**3:20 PM** **Break**

**3:40 PM** **Use of Molecular Dynamics and Quantum Methods in Aerospace:** *Sam Tucker*<sup>1</sup>; <sup>1</sup>Boeing

**4:00 PM** **Effects of Heterogeneities on Recrystallization Kinetics and on Mechanical Properties of Partially Recrystallized Copper: Experiments and Modelling:** *Fengxiang Lin*<sup>1</sup>; Yubin Zhang<sup>1</sup>; Dorte Juul Jensen<sup>1</sup>; <sup>1</sup>Technical University of Denmark

**4:20 PM** **A Continuum Dislocation Dynamics Approach to Crystal Plasticity of Two-phase Titanium Alloys:** *Hector Basoalto*<sup>1</sup>; Jeffery Brooks<sup>1</sup>; <sup>1</sup>University of Birmingham

**Modeling at Different Scales IV • Room: Arkansas/Platte**

**Invited**  
**2:00 PM** **PRISMS: An Integrated Predictive Multi-Scale Capability for the Materials Community:** *John Allison*<sup>1</sup>; Larry Aagesen<sup>1</sup>; Samantha Daly<sup>1</sup>; Krishna Garikipati<sup>1</sup>; Vikram Gavini<sup>1</sup>; Margaret Hedstrom<sup>1</sup>; H. V. Jagadish<sup>1</sup>; J. Wayne Jones<sup>1</sup>; Emmanuelle Marquis<sup>1</sup>; Brian Puchala<sup>1</sup>; Shiva Rudraraju<sup>1</sup>; Veera Sundararaghavan<sup>1</sup>; Sravya Tamma<sup>1</sup>; Glenn Tarcea<sup>1</sup>; Katsuyo Thornton<sup>1</sup>; Anton Van der Ven<sup>2</sup>; <sup>1</sup>The University of Michigan; <sup>2</sup>University of California Santa Barbara

**Invited**  
**2:20 PM** **Bottom-up and Top-down Uncertainty Quantification of bcc Fe Single Crystal Plasticity:** *Aaron Tallman*<sup>1</sup>; Joel Blumer<sup>1</sup>; Yan Wang<sup>1</sup>; Sankar Narayanan<sup>1</sup>; Ting Zhu<sup>1</sup>; David McDowell<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

**2:40 PM** **Phase-Field Simulations of Precipitation in an Mg-Nd Alloy:** *Larry Aagesen*<sup>1</sup>; Shiva Rudraraju<sup>1</sup>; Ellen Sitzmann<sup>1</sup>; Vicente Araullo-Peters<sup>1</sup>; Emmanuelle Marquis<sup>1</sup>; Katsuyo Thornton<sup>1</sup>; John Allison<sup>1</sup>; <sup>1</sup>University of Michigan

**3:00 PM** **A Multi-Scale Comparison of Grain Boundary Structure Using the Phase-Field Crystal Model and Molecular Dynamics:** *Jason Luce*<sup>1</sup>; Bradley Hodge<sup>2</sup>; Philip Goins<sup>2</sup>; Elizabeth Holm<sup>2</sup>; Katsuyo Thornton<sup>1</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>Carnegie Mellon University

**3:20 PM** **Break**

**3:40 PM** **Additive Manufacturing of Two-Phase Titanium Alloys: A Micro-Macro Scale Modelling Approach:** *Yogesh Sovani*<sup>1</sup>; Chinnapat Panwisawas<sup>1</sup>; Richard Turner<sup>1</sup>; Jeffery Brooks<sup>1</sup>; Hector Basoalto<sup>1</sup>; <sup>1</sup>University of Birmingham

**4:00 PM** **Computation of Effective Radiative Properties of Powders for Selective Laser Sintering Simulations:** *Daniel Moser*<sup>1</sup>; Sreekanth Pannala<sup>2</sup>; Jayathi Murthy<sup>1</sup>; <sup>1</sup>University of Texas at Austin; <sup>2</sup>Oak Ridge National Laboratory

**4:20 PM** **Multiscale Modeling of Thermal Protection Materials I: Atomistic Modeling of Constituent Properties:** *John Lawson*<sup>1</sup>; Joshua Monk<sup>1</sup>; Charles Bauschlicher<sup>1</sup>; Steven Arnold<sup>2</sup>; Pappu Murthy<sup>2</sup>; Brett Bednarcyk<sup>2</sup>; <sup>1</sup>NASA Ames Research Center; <sup>2</sup>NASA Glenn Research Center

**4:40 PM** **An Image-Based Finite Element Model for Ni-Based Superalloys Using a Two-Scale Constitutive Model:** *George Weber*<sup>1</sup>; Somnath Ghosh<sup>1</sup>; David Eastman<sup>1</sup>; Will Lenthe<sup>2</sup>; Kevin Hemker<sup>1</sup>; Tresa Pollock<sup>2</sup>; Chris Woodward<sup>3</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>University of California Santa Barbara; <sup>3</sup>U.S. Air Force Research Laboratory

5:00 PM **Electric Field and the Kinetics Characteristics of the Growth of a Metal Oxide Film at High Temperature - Insights from Diffuse-interface Modeling and Simulation:** *Tian-Le Cheng*<sup>1</sup>; *You-Hai Wen*<sup>1</sup>; *Jeffrey Hawk*<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory

## ICME Models, Tools and Infrastructure IV • Room: Rio Grande/Gunnison

2:00 PM **HPC in Experiment-Informed Materials Genome and Materials Design:** *Wing Liu*<sup>1</sup>; *Jacob Smith*<sup>1</sup>; <sup>1</sup>Northwestern University

2:20 PM **Extending CALPHAD Based Tools with Process-Structure-Property Models to Develop a Computational Materials Design Platform:** *Paul Mason*<sup>1</sup>; *Q. Chen*<sup>2</sup>; *A. Engstrom Engstrom*<sup>2</sup>; *K. Wu*<sup>1</sup>; <sup>1</sup>Thermo-Calc Software Inc.; <sup>2</sup>Thermo-Calc Software AB

2:40 PM **Phase-field Simulations of Aluminumization of Nickel-based Alloys during Pack Cementation:** *Stefan Poulsen*<sup>1</sup>; *Ashley Paz Y Puente*<sup>1</sup>; *Dinc Erdeniz*<sup>1</sup>; *Thomas Philippe*<sup>1</sup>; *Peter Voorhees*<sup>1</sup>; *David Dunand*<sup>1</sup>; <sup>1</sup>Northwestern University

3:00 PM **Phase Field Modeling of Recrystallization in Titanium-Aluminum Alloys:** *Susan Gentry*<sup>1</sup>; *Anna Trump*<sup>1</sup>; *John Allison*<sup>1</sup>; *Katsuyo Thornton*<sup>1</sup>; <sup>1</sup>University of Michigan

3:20 PM **Break**

3:40 PM **ICME Training in Materials Science and Engineering Curriculum:** *Lan Li*<sup>1</sup>; <sup>1</sup>Boise State University

4:00 PM **Micro-bending Fatigue Testing of Ni and Ni-base Superalloys: Experiments Supporting ICME:** *Zafir Alam*<sup>1</sup>; *Jessica Krogstad*<sup>2</sup>; *David Eastman*<sup>1</sup>; *Thomas Straub*<sup>3</sup>; *Christoph Eberl*<sup>3</sup>; *Kevin Hemker*<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>University of Illinois; <sup>3</sup>Fraunhofer Institute for Mechanics of Materials

4:20 PM **Expanding Dynamic Data Evaluation to Metals and Alloys:** *Boris Wilthan*<sup>1</sup>; *Vladimir Diky*<sup>1</sup>; *Erik Pfeifl*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

4:40 PM **The Role of Path Sequencing on Additive Manufacturing: Effect on Phase Change Dynamics and Heat Transfer:** *Sreekanth Pannala*<sup>1</sup>; *Srdjan Simunovic*<sup>1</sup>; *Naren Raghavan*<sup>2</sup>; *Neil Carlson*<sup>3</sup>; *Suresh Babu*<sup>4</sup>; *John Turner*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>Oak Ridge National Laboratory/University of Tennessee Knoxville; <sup>3</sup>Los Alamos National Laboratory; <sup>4</sup>University of Tennessee Knoxville

## Thursday, June 4, 2015

### Plenary Session IV • Room: Colorado Ballroom II & III

8:00 AM **Invited Modeling Across Length Scales: A Roadmapping Study:** *Peter Voorhees*<sup>1</sup>; *George Spanos*<sup>2</sup>; <sup>1</sup>Northwestern University; <sup>2</sup>The Minerals, Metals & Materials Society (TMS)

8:30 AM **Invited NIST and Materials Genome Initiative:** *James Warren*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

8:50 AM **Invited ICME-Related Opportunities at the National Science Foundation:** *Alexis Lewis*<sup>1</sup>; <sup>1</sup>National Science Foundation

9:10 AM **Break**

9:20 AM **Invited Rectifying Bottom-up and Top-down Uncertainties in Multiscale Modeling:** *David McDowell*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

9:50 AM **Invited Microstructure Modelling in ICME Settings:** *Georg Schmitz*<sup>1</sup>; *Markus Apel*<sup>1</sup>; *Bernd Böttger*<sup>1</sup>; <sup>1</sup>Access RWTH Aachen

10:10 AM **Break**

10:30 AM **Panel Discussion**

11:30 AM **Concluding Comments**





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