

9:30 AM

Study of Metallic Calibrated Defects by Subsurface Nanoscale Imaging: *Pauline Vitry*¹; Laurène Tétard²; Eric Bourillot¹; Cédric Plassard¹; Yvon Lacroute¹; Eric Lesniewska¹; ¹University of Bourgogne; ²University of Central Florida

9:50 AM

Effective Measurement of Elastic Constants from Polycrystalline Samples: *Xinpeng Du*¹; Peng Zhao¹; Ji-Cheng Zhao¹; ¹The Ohio State University

10:10 AM Break

10:20 AM

Interface-Driven Plasticity: The Presence of an Interface Affected Zone in Metallic Lamellar Composites: *John Carpenter*¹; Rodney McCabe¹; Jason Mayeur¹; Nathan Mara¹; Irene Beyerlein¹; ¹Los Alamos National Laboratory

10:40 AM

Investigation of Strain Transfer Across Grain Boundaries in Commercially Pure Tantalum: *Bret Dunlap*¹; Philip Eisenlohr¹; Claudio Zambaldi²; David Mercier²; Yang Su¹; Thomas Bieler¹; Martin Crimp¹; ¹Michigan State University; ²Max-Planck-Institut für Eisenforschung

11:00 AM

Innovative Procedure for the Characterisation of Thermo-mechanical Properties Of Carbon Base Materials Using The Gleeble® 3800 System: *Dany Racine*¹; Dmitry Lukovnikov¹; Daniel Marceau¹; Denis Laroche²; ¹University Research Centre on Aluminium (CURAL) - Aluminium Research Centre (REGAL) - University of Québec at Chicoutimi; ²Rio Tinto Alcan (Arvida Research and Development Center)

11:20 AM

Solid Solution Characterization in Metal by Original Tomographic Scanning Microwave Microscopy Technique: *Eric Bourillot*¹; Pauline Vitry¹; Virgil Optasanu¹; Tony Montessin¹; Eric Lesniewska¹; ¹University of Bourgogne

11:40 AM

Real Space Measurement of Lattice Misfit with Scanning Transmission Electron Microscopy: *Adedapo Oni*¹; Xiahan Sang¹; Santoshrupa Dumpala²; Selva Raju³; Aakash Kumar⁴; Srikant Srinivasan²; Scott Broderick²; Surendra Saxena²; Susan Sinnott⁴; Krishan Rajan²; James LeBeau¹; ¹North Carolina State University; ²Iowa State University; ³Florida International University; ⁴University of Florida

Computational Modeling and Stochastic Methods for Materials Discovery and Properties – Stochastic, Statistic, and Multiscale Methods

Sponsored by: TMS Functional Materials Division (formerly EMPMD), TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Richard Hennig, University of Florida; Francesca Tavazza, National Institute of Standards and Technology; Dallas Trinkle, University of Illinois at Urbana-Champaign; Mikhail Mendelev, Ames Laboratory; Adri van Duin, Pennsylvania State University

Tuesday AM

March 17, 2015

Room: Northern Hemisphere A4

Location: Dolphin

Session Chair: Adri van Duin, Pennsylvania State University

8:30 AM

Atoms-to-Continuum Simulation of the Rapid Solidification of Metallic Liquids: *Howard Sheng*¹; ¹GMU

8:50 AM

Computer Simulation of Martensite Spread: A Stochastic Approach: *Paulo Rios*¹; Filipi Cardoso¹; Matheus Nogueira¹; Tiago Neves¹; José Roberto Guimarães¹; ¹UFF-EIIMVR

9:10 AM

Grain Network Representation of Microstructure: Predicting Rare Microstructural Events: *Brian DeCost*¹; Elizabeth Holm¹; ¹Carnegie Mellon University

9:30 AM

Kinetic Monte Carlo Enabled Modeling of Diffusion Assisted Plastic Deformation: *James Martino*¹; Srinath Chakravarthy¹; ¹Northeastern University

9:50 AM Break

10:05 AM

Modeling Chemical Fluctuations Across Stacking Faults in L12-Containing Co-base Superalloys Using Cluster-Assisted Statistical Mechanics: *Michael Titus*¹; Robert Rhein¹; Philip Dodge¹; Alessandro Mottura¹; Anton Van der Ven¹; Tresa Pollock¹; ¹University of California, Santa Barbara

10:25 AM

Modeling Stress Corrosion Cracking in Metals and Alloys: *Tahir Cagin*¹; Hieu Pham¹; Richard Gustafson¹; ¹Texas A&M University

10:45 AM

Obtaining a Bimodal Grain Size Distribution via Thermal Treatment for Property Optimization: *David Wu*¹; Hao Yuan Tay¹; Muhammad Huzaifah¹; Siu Sin Quek¹; ¹Institute of High Performance Computing, A*STAR

11:05 AM

Parameter Estimation in Mechanistic Tool Wear Model: A Bayesian Approach: *Farbod Akhavan Niaki*¹; Durul Ulutan¹; Laine Mears¹; ¹Clemson University

11:25 AM

Thermally-Activated Non-Schmid Glide of Screw Dislocations in W Using Atomistically-Informed Kinetic Monte Carlo Simulations: Alexander Stukowski¹; David Cereceda²; Thomas Swinburne³; *Jaime Marian*²; ¹Darmstadt University of Technology; ²University of California Los Angeles; ³Imperial College

Computational Thermodynamics and Kinetics – Grain Boundary and Grain Growth

Sponsored by: TMS Functional Materials Division (formerly EMPMD), TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee, TMS: Computational Materials Science and Engineering Committee

Program Organizers: Richard Hennig, University of Florida; Francesca Tavazza, National Institute of Standards and Technology; Maryam Ghazisaeidi, The Ohio-State University; Vidvuds Ozolins, University of California Los Angeles

Tuesday AM

March 17, 2015

Room: Oceanic 3

Location: Dolphin

Session Chair: Dallas Trinkle, University of Illinois, Urbana-Champaign

8:30 AM

Atomistic Modeling of Pre-Melted Grain Boundaries: *J. Hickman*¹; Y. Mishin¹; ¹George Mason University

8:50 AM

Atomistic Simulations of Grain Boundary Mobilities in the Iron-Helium System: *Tegar Wicaksono*¹; Chad Sinclair¹; Matthias Miltzer¹; ¹The University of British Columbia

9:10 AM

Computational Study of the Stiffness of Asymmetric Tilt Boundaries in a Model Bcc Binary Alloy: *Isaac Toda-Caraballo*¹; Paul Bristowe¹; ¹University of Cambridge

9:30 AM Invited

Grand-Canonical Thermodynamics of Grain Boundaries: *Danny Perez*¹; Thomas Vogel¹; Blas Uberuaga¹; ¹Los Alamos National Laboratory